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(54) Title: CRYSTALLIZED P38 COMPLEXES

(57) Abstract

This invention provides certain crystallized, protein kinase–ligand complexes, in particular P38–ligand complexes, and their structure coordinates. The structure coordinates are based on the structure of a phosphorylated P38γ complex which has now been solved and which reveals new structural information useful for understanding the activated states of other, related kinase proteins as described herein. The key structural features of the proteins, particularly the shape of the substrate binding site, are useful in methods for designing or identifying selective inhibitors of the protein kinases, particularly P38γ and in solving the structures of other proteins with similar features. The structure coordinates may be encoded in a data storage medium for use with a computer for graphical three–dimensional representation of the structure and for computer–aided molecular design of new inhibitors.

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CRYSTALLIZED P38 COMPLEXES

TECHNICAL FIELD OF INVENTION

This application claims priority from U.S. Provisional Applications Serial No. 60/112,354 filed December 16, 1998, U.S. Provisional Application Serial No. 60/163,373 filed November 3, 1999

This invention relates to certain crystallized kinase protein-ligand complexes, particularly complexes of crystallized P38 protein, and more particularly complexes of P38γ protein. This invention also relates to crystallizable compositions from which the protein-ligand complexes may be obtained. This invention also relates to computational methods of using structure coordinates of the protein complex to screen for and design compounds that interact with the protein, particularly P38 protein or homologues thereof.

BACKGROUND OF THE INVENTION

Mammalian cells respond to extracellular stimuli by activating signaling cascades that are mediated by members of the mitogen-activated protein (MAP) kinase family. Mammalian mitogen-activated protein (MAP) kinases are proline-directed serine/threonine kinases that facilitate signal translocation in cells [Davis, *Mol. Reprod. Dev.* 42, 459-467 (1995); Cobb et al., *J. Biol. Chem.* 270, 14843-14846 (1995); Marshall, *Cell* 80, 179-185 (1995)]. MAP kinases include the extracellular-signal regulated kinases (ERKs), the c-Jun NH_2-terminal kinases (JNKs) and the P38 kinases, which have similar sequences and three-dimensional structures [Taylor &

Radzio-Andzlem (1994); *Structure* 2, 345-355; Kultz *J Mol Evol* 46, 571-588 (1998)].

Activation of the MAPK P38α has been observed in cells stimulated by stresses, such as treatment by lipopolysaccharides (LPS), UV, anisomycin, or osmotic shock, and by cytokines, such as interleukin-1 (IL-1) and tissue necrosis factor (TNF). Inhibition of P38α kinase leads to a blockade on the production of both IL-1 and TNF. IL-1 and TNF stimulate the production of other proinflammatory cytokines such as IL-6 and IL-8 and have been implicated in acute and chronic inflammatory diseases and in post-menopausal osteoporosis [Kimble et al., *Endocrinol.*, 136, 3054-61 (1995)].

Based upon this finding it is believed that P38α, along with other MAPKs, has a role in mediating cellular response to inflammatory stimuli, such as leukocyte accumulation, macrophage/monocyte activation, tissue resorption, fever, acute phase responses and neutrophilia. In addition, the MAPKs, such as P38α, have been implicated in cancer, thrombin-induced platelet aggregation, immunodeficiency disorders, autoimmune diseases, cell death, allergies, osteoporosis and neurodegenerative disorders. Inhibitors of P38α also appear to be involved in pain management through inhibition of prostaglandin endoperoxide synthase-2 induction. Other diseases associated with Il-1, IL-6, IL-8 or TNF overproduction are set forth in WO 96/21654. P38γ MAP kinase (also known as ERK6 and stress activated protein kinase-3 or SAPK3) is a newly discovered member of the MAP kinase family. However, unlike the other P38 family members which are expressed in many tissues, P38γ is expressed at highest levels in skeletal muscle [Li et al., *Biochem Biophys Res Commun* 228, 334-340 (1996);

Enslen et al., *J Biol Chem* 273, 1741-1748 (1998); Raingeaud et al., *J. Biol. Chem.* 270, 7420-7426 (1995)]. Thus P38γ may have a unique function related to muscle morphogenesis, and it may be a potential target for treating degenerative diseases occurring in muscle tissue.

Compounds that selectively inhibit P38γ and not P38α would be highly desirable. It would be useful to have new treatments for muscle degenerative diseases using compounds that do not suppress the inflammatory response or other functions of P38α. However, the design of inhibitors that are selective for any particular MAP kinase, such as P38γ, is challenging due to the structural similarity of the MAP kinases. Therefore, it would be advantageous to have a detailed understanding of the structures of the various MAP kinases in order to exploit any subtle differences that may exist among them.

A general approach to designing inhibitors that are selective for an enzyme target is to determine how a putative inhibitor interacts with the three dimensional structure of the enzyme. For this reason it is useful to obtain the enzyme protein in crystal form and perform X-ray diffraction techniques to determine its three dimensional structure coordinates. If the enzyme is crystallized as a complex with a ligand, one can determine both the shape of the enzyme binding pocket when bound to the ligand, as well as the amino acid residues that are capable of close contact with the ligand. By knowing the shape and amino acid residues in the binding pocket, one may design new ligands that will interact favorably with the enzyme. With such structural information, available computational methods may be used to predict how strong the ligand binding interaction will

be. Such methods thus enable the design of inhibitors that bind strongly, as well as selectively to the target enzyme.

Crystal structures are known for some of the MAP kinases; for example, unphosphorylated JNK3, unphosphorylated P38α, and ERK2 in both phosphorylated and unphosphorylated forms. Phosphorylated ERK2 is reported to exist as a dimer in both solution and as a crystal. The unphosphorylated forms of JNK3, ERK2 and P38α, on the other hand, are reported to be monomeric. [Tong et al., *Nat Struct Biol* 4, 311-316 (1997); Wilson and Su, *Chem Biol* 4, 423-431 (1997); Xie et al., *Structure* 6, 983-991 (1998); Zhang et al., *Nature* 367, 704-711 (1994); Canagarajah et al., *Cell* 90, 859-869 (1997); Wilson and Su, *J Biol Chem* 271, 27696-27700 (1996)]

The crystal structure reported for P38α is based on unphosphorylated protein. However, it is the phosphorylated or activated form of the enzyme that is able to phosphorylate its substrate enzyme. In order to disrupt the phosphorylation of the substrate, and produce the desired clinical effect, a small molecule inhibitor would likely act by blocking a phosphorylated form of P38. Thus, the most suitable target for drug design is the active or phosphorylated form. While the structure of the unphosphorylated enzyme is often used for drug design purposes, there is an inherent uncertainty as to whether the phosphorylated and unphosphorylated forms would bind a designed inhibitor with equal affinity.

A class of pyridinylimidazole compounds are known to inhibit P38α MAP kinase [Lee et al., *Nature* 372, 739-746 (1994)]. These inhibitors have been shown to bind in the

ATP binding site of P38α [Young et al., *J Biol Chem* 272, 12116-12121 (1997); Tong et al., *Nat Struct Biol* 4, 311-316 (1997); Wilson et al., *Chem Biol* 4, 423-431 (1997)]. However, the pyridinylimidazoles reportedly do not inhibit the activity of ERK2, JNK3, or P38γ. This observed selectivity is interesting because the amino acid sequence in the ATP binding site of the various kinases are known to be highly conserved [Fox et al., *Protein Science* 7, 2249-2255 (1998); Xie et al., supra; Wilson and Su, supra; Enslen et al., *J Biol Chem* 273, 1741-1748 (1998)].

As there is a need for compounds that selectively inhibit a particular MAP kinase, it would be desirable to have improved methods that facilitate the design of such compounds. For this purpose, knowledge of the three dimensional structure coordinates of an activated P38 protein would be useful. Such information would aid in identifying and designing potential inhibitors of particular P38 proteins which, in turn, are expected to have therapeutic utility.

SUMMARY OF THE INVENTION

This invention provides certain crystallized, protein kinase-ligand complexes, in particular P38-ligand complexes, and their structure coordinates. The structure coordinates are based on the structure of a phosphorylated P38γ-ligand complex that has now been solved and which reveals new structural information useful for understanding the activated states of other, related kinase proteins as described herein. The key structural features of the proteins, particularly the

shape of the substrate binding site, are useful in methods for designing or identifying selective inhibitors of the protein kinases, particularly P38, and in solving the structures of other proteins with similar features.

The invention also provides a computer which which is programmed with the structure coordinates of the activated P38 binding site. Such a computer, appropriately programmed and attached to the necessary viewing device, is capable of displaying a three-dimensional graphical representation of a molecule or molecular complex comprising such binding sites or similarly shaped homologous binding pockets.

The invention also provides a method for determining at least a portion of the three-dimensional structure of other molecules or molecular complexes which contain at least some features that are structurally similar to P38γ, particularly P38α, P38β, P38δ and other P38 isoforms. This is achieved by using at least some of the structural coordinates obtained for a phosphorylated P38 complex.

BRIEF DESCRIPTION OF THE FIGURES

Figure 1 lists the atomic structure coordinates for phosphorylated P38γ in complex with MgAMP-PNP as derived by X-ray diffraction from a crystal of that complex. The following abbreviations are used in Figure 1:

"Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

"X, Y, Z" crystallographically define the atomic position of the element measured.

"B" is a thermal factor that measures movement of the

atom around its atomic center.

"Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

Fig 1a is an overview of the phosphorylated P38γ.

Fig 2 is a superimposition of unphosphorylated P38γ and phosphorylated P38γ.

Fig 3 is a detailed stereo view of the activation loop.

Fig 4 is a stereo view of the AMP-PNP bound in the active site.

Fig 5 is a comparison of the active sites of activated P38γ with P38α (a) and cAPK or cyclic AMP dependent protein kinase(b).

Fig 6 is a comparison of activated phosphorylation loops from P38γ (dark orange), ERK2 (dark blue), and cAPK (red).

Figure 7 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figures 8 and 9.

Figure 8 shows a cross section of a magnetic storage medium.

Figure 9 shows a cross section of a optically-readable data storage medium.

DETAILED DESCRIPTION OF THE INVENTION

This invention provides certain crystallized, protein kinase-ligand complexes, in particular P38-ligand complexes, and their structure coordinates. The

structure coordinates are based on the structure of a phosphorylated P38γ complex that has now been solved and which reveals new structural information regarding the activated states of other, related kinase proteins as described herein. The key structural features of the protein, particularly the shape of the substrate binding site, are useful in methods for designing inhibitors of the P38 and in solving the structures of other proteins with similar features.

In describing protein structure and function, reference is made to amino acids comprising the protein. The amino acids may also be referred to by their conventional abbreviations, as shown in the table below.

A =	Ala =	Alanine	T =	Thr =	Threonine
V =	Val =	Valine	C =	Cys =	Cysteine
L =	Leu =	Leucine	Y =	Tyr =	Tyrosine
I =	Ile =	Isoleucine	N =	Asn =	Asparagine
P =	Pro =	Proline	Q =	Gln =	Glutamine
F =	Phe =	Phenylalanine	D =	Asp =	Aspartic Acid
W =	Trp =	Tryptophan	E =	Glu =	Glutamic Acid
M =	Met =	Methionine	K =	Lys =	Lysine
G =	Gly =	Glycine	R =	Arg =	Arginine
S =	Ser =	Serine	H =	His =	Histidine

This invention also provides a crystallizable composition from which the crystallized protein is obtained. The crystallizable composition preferably comprises a phosphorylated P38 protein complexed with a substrate or ligand. The ligand may be any ligand capable of binding to the P38 protein, and is preferably

a ligand that binds to the ATP binding site of the protein. Examples of such ligands are small molecule inhibitors of the particular P38 as well as non-hydrolyzable ATP analogs and suicide substrates. Non-hydrolyzable ATP analogs useful in the crystallizable compositions of this invention include AMP-PCH_2P, AMP-PSP and AMP-PNP where the oxygen linking the second and third phosphates of the ATP analogs is replaced by CH_2, S and NH, respectively. An example of a suicidal substrate is 5'-(p-fluorosulfonyl benzoyl)adenosine (FSBA). Preferably, the crystallizable compositions of this invention comprise AMP-PNP as the substrate. It is preferred that the composition further comprise divalent cations, especially magnesium or magnanese cations, which may be introduced in any suitable manner. For example, the cations may be introduced by incubating the desired ligand with a suitable metal salt such as $MgCl_2$ prior to incubation with the phosphorylated P38 protein.

It has been found that the crystallization of the phosphorylated P38 protein is sensitive to buffer conditions. Thus, in a preferred embodiment, the crystallizable compositions of this invention further comprise a suitable glycol such as ethylene glycol, polyethylene glycol (PEG), PEG-monomethyl ether or mixtures thereof, preferably PEG 4000, as an aqueous solution containing between about 10 to 35% of the glycol by volume of solution, a salt, such as sodium acetate at about 50 to 200 mM, a reducing agent, such as dithiothreitol (DTT) at between about 1 to 10 mM, a detergent such as C12E9 at about 0.01 to 0.05%, and a buffer that maintains pH at between about 8.0 and 9.0. An example of a suitable buffer is 100 mM Tris at pH 8.5.

By applying standard crystallization protocols to the

above described crystallizable compositions, crystals of the phosphorylated P38 protein complex may be obtained. Thus, one aspect of this invention relates to a method of preparing phosphorylated P38-containing crystals. The method comprises the steps of

(a) obtaining a crystallizable composition comprising a phosphorylated P38 protein, divalent cations, and a ligand capable of binding to the protein, and

(b) subjecting the composition of step (a) to conditions which promote crystallization.

Figure 1 shows the structure coordinates of a phosphorylated P38γ protein complexed with MgAMP-PNP. The manner of obtaining these structure coordinates, interpretation of the coordinates and their utility in understanding the protein structure, as described herein, will be understood by those of skill in the art and by reference to standard texts such as Crystal Structure Analysis, Jenny Pickworth Glusker and Kenneth N. Trueblood, 2nd Ed. Oxford University Press, 1985, New York; and Principles of Protein Structure, G.E. Schulz and R.H. Schirmer, Springer-Verlag, 1985, New York.

Those of skill in the art understand that a set of structure coordinates for an enzyme or an enzyme-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with

those pockets.

These variations in coordinates may be generated because of mathematical manipulations of the P38γ/MgAMP-PNP structure coordinates. For example, the structure coordinates set forth in Figure 1 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same. Thus, for example, a ligand that bound to the active site binding pocket of P38γ would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the acceptable error.

The term "binding pocket" refers to a region of the protein that, as a result of its shape, favorably associates with a ligand or substrate. The term "P38γ-like binding pocket" refers to a portion of a molecule or molecular complex whose shape is sufficiently similar to the P38γ binding pockets as to bind common ligands. This commonality of shape may be quantitatively defined by a root mean square deviation (rmsd) from the structure coordinates of the backbone atoms of the amino acids that make up the binding pockets in P38γ (as set forth in Figure 1). The method of performing this rmsd

calculation is described below.

The "active site binding pockets" or "active site" of P38γ refers to the area on the P38γ enzyme surface where the substrate binds. In resolving the crystal structure of phosphorylated P38γ in complex with MgAMP-PNP, applicants have determined that P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 are within 5Å of and therefore close enough to interact with MgAMP-PNP. These amino acids are hereinafter referred to as the "**SET 5A amino acids.**" Thus, a binding pocket defined by the structural coordinates of those amino acids, as set forth in Figure 1; or a binding pocket whose root mean square deviation from the structure coordinates of the backbone atoms of those amino acids of not more than about 1.15 angstroms (Å) is considered a P38γ-like binding pocket of this invention.

Applicants have also determined that in addition to the P38γ amino acids set forth above, Pro32, Cys42, Ser43, Val53, Ile55, Lys57, Leu58, Thr59, Arg70, Glu74, Gly88, Leu107, Val108, Leu116, Gly117, Pro156, Leu159, Val161, Lys168, Phe172, Ala175, and Thr188 are within 8Å of bound MgAMP-PNP and therefore are also close enough to interact with that substrate. These amino acids, in addition to the SET 5A amino acids, are hereinafter referred to as the "**SET 8A amino acids.**" Thus, in a preferred embodiment, a binding pocket defined by the structural coordinates of the amino acids within 8Å of bound MgAMP-PNP, as set forth in Figure 1; or a binding pocket whose root mean square deviation from the structure coordinates of the backbone atoms of those

amino acids of not more than about 1.15Å is considered a preferred P38γ-like binding pocket of this invention.

It will be readily apparent to those of skill in the art that the numbering of amino acids in other isoforms of P38 may be different than that set forth for P38γ. Corresponding amino acids in other isoforms of P38 are easily identified by visual inspection of the amino acid sequences or by using commercially available homology software programs, as further described below.

Various computational analyses may be used to determine whether a protein or the binding pocket portion thereof is sufficiently similar to the P38γ binding pockets described above. Such analyses may be carried out in well known software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

For the purpose of this invention, a rigid fitting method was conveniently used to compare protein structures. Any molecule or molecular complex or binding pocket thereof having a root mean square deviation of conserved residue backbone atoms (N, Cα, C, O) of less than about 1.15Å when superimposed on the relevant backbone atoms described by structure coordinates listed in Figure 1 are considered identical. More preferably, the root mean square deviation is less than about 1.0Å.

The P38 X-ray coordinate data, when used in conjunction with a computer programmed with software to translate those coordinates into the 3-dimensional structure of p38γ may be used for a variety of purposes, especially for purposes relating to drug discovery. Such software for generating three-dimensional graphical

representations are known and commercially available. The ready use of the coordinate data requires that it be stored in a computer-readable format. Thus, in accordance with the present invention, data capable of being displayed as the three dimensional structure of P38γ and portions thereof and their structurally similar homologues is stored in a machine-readable storage medium, which is capable of displaying a graphical three-dimensional representation of the structure.

Therefore, another embodiment of this invention provides a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when used by a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of the P38γ SET 5A amino acids, or preferably the P38γ SET 8A amino acids, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than about 1.15Å.

Even more preferred is a machine-readable data storage medium that is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex that is defined by the structure coordinates of all of the amino acids in Figure 1 or a homologue of said molecule or molecular complex, wherein said homologue has a root mean square deviation from the backbone atoms of all of the amino acids in Figure 1 of not more than about 1.15Å.

According to an alternate embodiment, the machine-readable data storage medium comprises a data storage

material encoded with a first set of machine readable data which comprises the Fourier transform of the structure coordinates set forth in Figure 1, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of another molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

For example, the Fourier transform of the structure coordinates set forth in Figure 1 may be used to determine at least a portion of the structure coordinates of other P38s, such as P38β, and P38δ and isoforms of P38β, P38δ or P38γ. The structure coordinates in Figure 1 and the Fourier transform of the coordinates are especially useful for determining the coordinates of other P38s in phosphorylated form.

According to an alternate embodiment, this invention provides a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by the P38γ SET 5A amino acids, or preferably the P38γ SET 8A amino acids, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å, wherein said computer comprises:

(a) a machine readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said machine readable data comprises the structure coordinates of P38γ or portions thereof;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium, for processing said machine-readable data into said three-dimensional representation; and

(d) an output hardware coupled to said central processing unit, for receiving said three Dimensional representation.

Figure 7 demonstrates one version of these embodiments. System 10 includes a computer 11 comprising a central processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bi-directional system bus 50.

Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 36 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a

graphical representation of a binding pocket of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

In operation, CPU 20 coordinates the use of the various input and output devices 36, 46 coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system 10 are included as appropriate throughout the following description of the data storage medium.

Figure 8 shows a cross section of a magnetic data storage medium 100 which can be encoded with a machine-readable data that can be carried out by a system such as system 10 of Figure 7. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24. The magnetic domains of coating 102 of medium 100 are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system 10 of Figure 7.

Figure 9 shows a cross section of an optically-readable data storage medium 110 which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system 10 of Figure 7. Medium 110 can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium 100 preferably has a suitable substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which preferably is substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

As mentioned above, the P38γ X-ray coordinate data is useful for screening and identifying drugs that inhibit P38, especially phosphorylated P38. For example, the structure encoded by the data may be computationally evaluated for its ability to associate with putative

substrates or ligands. Such compounds that associate with p38γ may inhibit p38γ, and are potential drug candidates. Additionally or alternatively, the structure encoded by the data may be displayed in a graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with the compounds.

Thus, according to another embodiment, this invention relates to a method for evaluating the potential of a compound to associate with a molecule or molecular complex comprising a binding pocket defined by the structure coordinates of the P38γ SET 5A amino acids, or preferably the P38γ SET 8A amino acids, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than about 1.15Å.

This method comprises the steps of:

a) creating a computer model of the binding pocket using structure coordinates wherein the root mean square deviation between said structure coordinates and the structure coordinates of the P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1 is not more than about 1.15 Å;

b) employing computational means to perform a fitting operation between the chemical entity and said computer model of the binding pocket; and

c) analyzing the results of said fitting operation

to quantify the association between the chemical entity and the binding pocket model.

The term "chemical entity", as used herein, refers to chemical compounds or ligands, complexes of at least two chemical compounds, and fragments of such compounds or complexes.

Even more preferably, the method evaluates the potential of a chemical entity to associate with a molecule or molecular complex defined by the structure coordinates of all of the P38γ amino acids, as set forth in Figure 1, or a homologue of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å.

Alternatively, the structural coordinates of the P38γ binding pocket can be utilized in a method for identifying a potential agonist or antagonist of a molecule comprising a P38γ-like binding pocket. This method comprises the steps of:

(a) using atomic coordinates of the P38γ SET 5A amino acids ± a root mean square deviation from the backbone atoms of said amino acids of not more than about 1.15Å, to generate a three-dimensional structure of molecule comprising a P38γ-like binding pocket;

(b) employing said three-dimensional structure to design or select said potential agonist or antagonist;

(c) synthesizing said agonist or antagonist; and

(d) contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

More preferred is the use of the atomic coordinates of the P38γ SET 8A amino acids, ± a root mean square

deviation from the backbone atoms of said amino acids of not more than 1.15Å, to generate a three-dimensional structure of molecule comprising a p38γ-like binding pocket. Most preferred is when the atomic coordinates of all the amino acids of P38γ according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å, are used to generate a three-dimensional structure of molecule comprising a P38γ-like binding pocket.

For the first time, the present invention permits the use of molecular design techniques to identify, select or design potential inhibitors of p38, based on the structure of a phosphorylated p38γ-like binding pocket. Such a predictive model is valuable in light of the high costs associated with the preparation and testing of the many diverse compounds that may possibly bind to the p38 protein.

According to this invention, a potential p38 inhibitor may now be evaluated for its ability to bind a P38γ-like binding pocket prior to its actual synthesis and testing. If a proposed compound is predicted to have insufficient interaction or association with the binding pocket, preparation and testing of the compound is obviated. However, if the computer modeling indicates a strong interaction, the compound may then be obtained and tested for its ability to bind. Testing to confirm binding may be performed using assays such as described in Example 6.

A potential inhibitor of a P38γ-like binding pocket may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the P38γ-like binding pockets.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a P38γ-like binding pocket. This process may begin by visual inspection of, for example, a P38γ-like binding pocket on the computer screen based on the P38γ structure coordinates in Figure 1 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined above. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities.

These include:

1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (A. Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, San Diego, CA.

3. AUTODOCK (D. S. Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

Once suitable chemical entities or fragments have been selected, they can be designed or assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of P38γ. This would be followed by manual model building using software such as Quanta or Sybyl [Tripos Associates, St. Louis, MO].

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989); G. Lauri and P. A. Bartlett, "CAVEAT: a Program to Facilitate the Design of Organic Molecules", J. Comput. Aided Mol. Des. , 8, pp. 51-66 (1994)). CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as ISIS (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992).

3. HOOK (M. B. Eisen et al, "HOOK: A Program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", Proteins: Struct., Funct., Genet., 19, pp. 199-221 (1994). HOOK is available from Molecular Simulations, San Diego, CA.

Instead of proceeding to build an inhibitor of a P38γ-like binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other P38γ binding compounds may be designed as a whole or "de novo" using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). There are many de novo ligand design

methods including:

1. LUDI (H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Molecular Simulations Incorporated, San Diego, CA.

2. LEGEND (Y. Nishibata et al., Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations Incorporated, San Diego, CA.

3. LeapFrog (available from Tripos Associates, St. Louis, MO).

4. SPROUT (V. Gillet et al, "SPROUT: A Program for Structure Generation)", J. Comput. Aided Mol. Design, 7, pp. 127-153 (1993)). SPROUT is available from the University of Leeds, UK.

Other molecular modeling techniques may also be employed in accordance with this invention [see, e.g., Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990); see also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992); L. M. Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in Reviews in Computational Chemistry, Vol. 5, K. B. Lipkowitz and D. B. Boyd, Eds., VCH, New York, pp. 337-380 (1994); see also, W. C. Guida, "Software For Structure-Based Drug Design", Curr. Opin. Struct. Biology,, 4, pp. 777-781 (1994)].

Once a compound has been designed or selected by the

above methods, the efficiency with which that entity may bind to a P38γ binding pocket may be tested and optimized by computational evaluation. For example, an effective P38γ binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient P38γ binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. P38γ binding pocket inhibitors may interact with the binding pocket in more than one of multiple conformations that are similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to a P38γ binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, PA ©1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, ©1995); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA ©1995); Insight II/Discover -

(Molecular Simulations, Inc., San Diego, CA ©1995); DelPhi (Molecular Simulations, Inc., San Diego, CA ©1995); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo^2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach enabled by this invention, is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a P38γ binding pocket. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy [E. C. Meng et al., *J. Comp. Chem.*, 13, 505-524 (1992)].

According to another embodiment, the invention provides compounds which associate with a P38γ-like binding pocket produced or identified by the method set forth above.

The structure coordinates set forth in Figure 1 can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex whose structure is unknown comprising the steps of:

a) crystallizing said molecule or molecular complex of unknown structure;

b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

c) applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown.

By using molecular replacement, all or part of the structure coordinates of the P38γ/MgAMP-PNP complex as provided by this invention (and set forth in Figure 1) can be used to determine the structure of another crystallized molecule or molecular complex more quickly and efficiently than attempting an ab initio structure determination.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the P38γ/MgAMP-PNP complex according to Figure 1 within the unit cell of the crystal of the

unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex [E. Lattman, "Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)].

The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the P38γ/MgAMP-PNP complex can be resolved by this method.

In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about another P38, such as P38α, P38β, P38δ, or isoforms of P38β, P38δ or P38γ. The structure coordinates of P38γ as provided by this invention are particularly useful in solving the structure of other isoforms of P38γ or P38γ complexes.

Furthermore, the structure coordinates of P38γ as provided by this invention are useful in solving the structure of P38γ proteins that have amino acid substitutions, additions and/or deletions (referred to collectively as "P38γ mutants", as compared to naturally occurring P38γ isoforms). These P38γ mutants may optionally be crystallized in co-complex with a chemical

entity, such as a non-hydrolyzable ATP analogue or a suicide substrate. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type p38γ. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions such as, for example, increased hydrophobic interactions, between P38γ and a chemical entity or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3A resolution X-ray data to an R value of about 0.22 or less using computer software, such as X-PLOR [Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)]. This information may thus be used to optimize known P38γ inhibitors, and more importantly, to design new P38γ inhibitors.

The structure coordinates described above may also be used to derive the dihedral angles, ϕ and ψ, that define the conformation of the amino acids in the protein backbone. As will be understood by those skilled in the art, the ϕ_n angle refers to the rotation around the bond between the alpha carbon and the nitrogen, and the ψ_n angle refers to the rotation around the bond between the carbonyl carbon and the alpha carbon. The subscript "n" identifies the amino acid whose conformation is being described [for a general reference, see Blundell and Johnson, Protein Crystallography, Academic Press, London, 1976].

Surprisingly, it has now been found that for the

crystalline P38γ-ligand complex, the conformation of Gly113 is very different from the conformations reported for corresponding amino acids in other protein kinases. In order to compare the conformations of P38γ and other protein kinases at a particular amino acid site, such as Gly113, along the polypeptide backbone well-known procedures may be used for doing sequence alignments of the amino acids. Such sequence alignments allow for the equivalent or corresponding sites to be compared. One such method for doing a sequence alignment is the "bestfit" program available from Genetics Computer Group which uses the local homology algorithm described by Smith and Waterman in *Advances in Applied Mathematics* 2; 482 (1981).

A suitable amino acid sequence alignment will require that the proteins being aligned share a minimum percentage of identical amino acids. Generally, a first protein being aligned with a second protein should share in excess of about 35% identical amino acids with the second protein. Hanks et al., *Science*, 241, 42 (1988); Hanks and Quinn, *Methods in Enzymology*, 200, 38 (1991).

Equivalents of the Gly113 residue of p38γ may also be identified by its functional position. Gly113 is the amino acid residue that immediately follows sequentially the amino acid residue that donates, or is capable of donating, a hydrogen bond to the N1 nitrogen of the adenosine ring of ATP or an ATP analog, if such ATP or ATP analog were to be in the binding pocket comprising the Gly113 residue. The ability of the amino acid to donate such a hydrogen bond occurs as the result of the spatial position of the amino acid in the binding pocket of the protein. As used herein, the term "corresponding amino acid" or "equivalent amino acid" refers to a

particular amino acid in a protein kinase that corresponds to another, particular amino acid in a different protein kinase as determined by sequence alignment and/or its functional position.

Table 1 shows the sequence alignments for selected protein kinases where corresponding amino acids are shown in the same column. The amino acid numbering is based on the assignments given in the Swiss-Prot database which is an international protein sequence database distributed by the European Bioinformatics Institute (EBI) in Geneva, Switzerland. The database can be found at www.ebi.ac.uk/swissprot. Erk6_HUMAN is the database protein name for P38γ. The ten amino acids immediately preceding G113 of P38γ are given starting with T103. Thus, for example, Gly113 of P38γ corresponds or is equivalent to the following: Gly110 of P38α (MP38_HUMAN), Glu107 of mouse ERK2, and Asp150 of human JNK3. The last column of Table 1 shows the Swiss-Prot database accession number.

Table 1. Sequence Alignments for Selected Proteins

Protein	Corresponding Amino Acid Sequences Using Swiss-Prot Amino Acid Numbering											Access Number
ERK6_HUMAN	T103	D	F	Y	L	V	M	P	F	M112	G113	P53778
MP38_HUMAN	N100	D	V	Y	L	V	T	H	L	M109	G110	Q16539
ERK2_HUMAN	K99	D	V	Y	I	V	Q	D	L	M108	E109	P28482
ERK2_MOUSE	K97	D	V	Y	I	V	Q	D	L	M106	E107	P27703
JNK3_HUMAN	Q140	D	V	Y	L	V	M	E	L	M149	D150	P53779
KAPA_MOUSE	S114	N	L	Y	M	V	M	E	Y	V123	A124	P05132
INSR_HUMAN	Q1097	P	T	L	V	V	M	E	L	M1106	A1107	P06213
LCK_HUMAN	E309	P	I	Y	I	I	T	E	Y	M318	E319	P06239
ZA70_HUMAN	E408	A	L	M	L	V	M	E	M	A417	G418	P43403
PKD1_DICDI	T107	K	I	H	F	I	M	E	Y	A116	G117	P34100
KPC1_YEAST	N898	R	I	Y	F	A	M	E	F	I907	G908	P24583
CLK1_HUMAN	G235	H	I	C	I	V	F	E	L	L244	G245	P49759
CLK2_HUMAN	G237	H	M	C	I	S	F	E	L	L246	G247	P49760
DOA_DROME	G243	H	M	C	I	V	F	E	M	L252	G253	P49762
DSK1_SCHPO	A160	H	V	C	M	V	F	E	V	L169	G170	P36616
MKK1_YEAST	S293	S	I	Y	I	A	M	E	Y	M302	G303	P32490
MKK2_YEAST	S286	S	I	Y	I	A	M	E	Y	M295	G296	P32491
NIMA_EMENI	Q83	D	L	Y	L	Y	M	E	Y	C92	G93	P11837
KMOS_HUMAN	S133	L	G	T	I	I	M	E	F	G142	G143	P00540
KC1A_HUMAN	D84	Y	N	V	L	V	M	D	L	L93	G94	P48729
KC1B_BOVIN	D84	Y	N	V	L	V	M	D	L	L93	G94	P35507
KC1D_HUMAN	D76	Y	N	V	M	V	M	E	L	L85	G86	P48730
CK11_YEAST	L136	H	N	I	L	V	I	D	L	L145	G146	P23291
CK12_YEAST	L143	H	N	I	L	V	I	D	L	L152	G153	P23292
HR25_YEAST	E76	Y	N	A	M	V	I	D	L	L85	G86	P29295
KNS1_YEAST	N387	H	I	C	L	V	T	D	L	Y396	G397	P32350
KYK1_DICDI	D1360	H	H	C	I	V	T	E	W	M1369	G1370	P18160
CKI1_SCHPO	L79	H	N	V	L	V	I	D	L	L88	G89	P40233
CDK2_HUMAN	N74	K	L	Y	L	V	F	E	F	L83	H84	P24941
KPBG_HUMAN	T97	F	F	F	L	V	F	D	L	M106	K107	Q16816

Protein	Corresponding Amino Acid Sequences Using Swiss-Prot Amino Acid Numbering											Access Number
KCC1_HUMAN	G89	H	L	Y	L	I	M	Q	L	V98	S99	Q14012

As noted above, the conformation of Gly113 is very different from the conformations reported for corresponding amino acids in other protein kinases. For Gly113 of the P38γ-AMPPNP complex, ψ_{112} was found to be about 24 degrees and ϕ_{113} was found to be about 96 degrees. Table 2 shows the dihedral angles for Met112 and Gly113 of P38γ-AMPPNP complex and how these angles compare to those of the corresponding amino acids in other MAP kinases whose crystal structures have been reported. The protein names for the known proteins are provided as their Protein Data Bank™ (pdb) accession numbers. The Protein Data Bank is an international repository for three dimensional structures and can be located at www.rcsb.org/pdb/.

Table 2. Dihedral Angles (in degrees) for Met112 and Gly113 and Equivalents in P38 and Other Protein Kinases

	Met 112		Gly 113	
Protein	ϕ	ψ	ϕ	ψ
P38γ-AMPPNP	-106.2	23.8	96.24	-90.6
P38α-ligand[a]	-80.8	-26.5	95.7	-22.5
1ERK[b]	-119.1	131.7	-51.6	-55.6
2ERK [c]	-99.5	130.3	-42.7	-49.9
1p38[d]	-92.7	128.4	-82.1	-103.2
1ATP[e]	-96.6	89.1	-56.1	-30.1
1JNK [f]	-105.3	170.6	-92.2	-22.8
1IR3[g]	-112.7	87.9	-44.2	-38.4
1IRK[h]	-85.6	109.9	-40.7	-38.4
3LCK[i]	-121.7	105.9	-53.3	-38.2

[a] in-house structure of complex with a designed inhibitor;

[b] unphosphorylated ERK, reported in *Nature*, 367, 704, (1994);

[c] phosphorylated ERK, *Cell*, 90, 859 (1997);

[d] unphosphorylated p38γ, *Proc. Nat. Acad. Science*, 94, 2327 (1997);

[e] cyclic AMP dependent protein kinase or cAPK, *Acta Crys. Sec. D*, 49, 362 (1993);

[f] unphosphorylated JNK3, *Structure*, 6, 983 (1998);

[g] insulin receptor tyrosine kinase, *Embo J.*, 16, 5572 (1997);

[h] insulin receptor tyrosine kinase, *Nature*, 372, 786, (1994);

[i] lymphocyte-specific kinase, *Nature*, 368, 764, (1994)

It is well-recognized that there will be some variability in the conformations of corresponding amino acids in similar or identical proteins when the protein crystallization and structure determination are repeated. This variability in the ϕ and ψ dihedral angles may be

approximated by reference to Ramachandran plots comparing the conformations obtained for two or more identical or similar proteins [Blundell and Johnson, Protein Crystallography, Academic Press, London, 1976]. It may be expected that the dihedral angles of equivalent amino acid residues in identical or similar proteins will vary as much as about 45° or more.

It should be noted that the amino acid numbering defined in the Protein Data Bank™ may be offset from the numbering given in the Swiss-Prot database. This offset, when it occurs, will be readily understood by those skilled in the art. Thus, the sequences of those proteins that are listed in both databases may be easily compared despite offsets in amino acid numbering that may occur. Examples of such offsets occur for INSR_HUMAN where A1107 according to Swiss-Prot numbering is the same as A1080 in the PDB database and for LCK_HUMAN where E319 according to Swiss-Prot numbering is the same as E320 by PDB numbering.

The ψ_{112} and ϕ_{113} dihedral angles of the P38γ-AMPPNP complex shown in Table 2 indicate that the conformation of Gly113 in this complex is "flipped" or rotated considerably relative to corresponding amino acids in other MAP kinases. Therefore, the structure coordinates of P38γ set forth in Figure 1 represent, inter alia, what is believed to be a conformation at Met 112 and Gly113 that had not been observed for other crystalline protein kinases, especially other MAP kinases.

Accordingly, another embodiment of this invention relates to a crystalline protein kinase-ligand complex, said kinase comprising amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by

functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, wherein the ψ angle of the residue corresponding to Met112 is in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 is in the range of about 30° to 150°. Preferably, the ψ angle of the crystalline protein kinase-ligand complex is in the range of about -45° to 45° and most preferably in the range of about -30° to 30°. Preferably, the ϕ angle is in the range of about 45° to 135°, and most preferably is in the range of about 60° to 120°. Examples of kinases that may provide such a crystalline protein kinase when complexed with a ligand are described by Hanks et al., *Science*, 241, 42 (1988) and Hanks and Quinn, *Methods in Enzymology*, 200, 38 (1991). Other examples of such kinases may be found at www.sdsc.edu/Kinases/pkr/pk_catalytic/pk_hanks_seq_align_long.html, where the kinases are listed with their corresponding sequence alignments.

Another embodiment of this invention relates to a crystalline protein kinase-ligand complex, said kinase selected from the proteins listed in Table 1, wherein the ψ angle of the residue corresponding to Met112 is in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 is in the range of about 30° to 150°. Preferably, the ψ angle of the crystalline protein kinase-ligand complex is in the range of about -45° to 45° and most preferably in the range of about -30° to 30°. Preferably, the ϕ angle is in the range of about 45° to 135°, and most preferably is in the range of about 60° to 120°.

Structural information regarding the conformation of the Met112 and Gly113 residues of the crystalline P38γ-

complex may be encoded in a machine-readable data storage medium as described above for encoding the other structural coordinates of the protein. Accordingly, another embodiment of this invention relates to a computer for producing a three-dimensional representation of an ATP binding site of a protein kinase-ligand complex, or portion thereof, wherein said computer comprises:

a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said machine-readable data comprises the structure coordinates of a kinase, or portion thereof, said kinase or portion thereof comprising amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, wherein the ψ angle of the residue corresponding to Met112 is in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 is in the range of about 30° to 150°;

b) a working memory for storing instructions for processing said machine-readable data;

c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium, for processing said machine readable data into said three-dimensional representation; and

d) an output hardware coupled to said central-processing unit, for receiving said three-dimensional representation. Preferably, the machine-readable data comprises the structure coordinates of a kinase, or portion thereof, said kinase comprising amino acid

residues corresponding to the Met112 and Gly113 amino acids of P38γ or corresponding to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, wherein the ψ angle is in the range of about -45° to 45° and most preferably in the range of about -30° to 30°, and the ϕ angle is in the range of about 45° to 135°, and most preferably in the range of about 60° to 120°. In a more preferred embodiment of this computer, the machine readable data comprises the structure coordinates of a crystalline protein kinase-ligand complex, or portion thereof, where said kinase is selected from a protein listed in Table 1.

For designing new compounds that associate with a protein kinase binding pocket, it is useful to employ information that includes the conformations of the Met112 and Gly113 residues, or their equivalents, along with other structural information regarding amino acids in the binding pocket. For example, to evaluate the ability of a chemical entity to bind to a protein kinase, the conformations of Met112 and Gly113, or equivalents, may be used along with structure coordinates of the backbone atoms of amino acids in the protein kinase binding pocket. These structure coordinates and the structure coordinates of the p38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1 should not differ by more than about 3.0 angstroms in root mean square deviation, preferably the root mean square deviation is within about 2.7 angstroms, and most preferably within about 2.5 angstroms. For example, the root mean square deviation between the structure coordinates of the p38γ amino acids

and those of a p38γ complex (see Table 2) was found by applicants to be 2.41 angstroms. Resolution error may account for variation in the root mean square deviation of a few tenths of an angstrom.

Accordingly, another embodiment of this invention provides a method for evaluating the ability of a chemical entity to associate with a protein kinase binding pocket, said method comprising the steps of:

a) creating a computer model of the binding pocket using structure coordinates wherein:

(i) the root mean square deviation between said structure coordinates and the structure coordinates of the P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1 is within about 3.0 angstroms,

(ii) said binding pocket model depicts amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, and

(iii) said binding pocket model depicts the ψ angle of the residue corresponding to Met112 to be in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 to be in the range of about 30° to 150°;

b) employing computational means to perform a fitting operation between the chemical entity and the binding pocket model; and

c) analyzing the results of said fitting operation to quantify the association between the chemical entity-

and the binding pocket model.

A useful root mean square deviation between the structure coordinates of a particular binding pocket and the structure coordinates of the binding pocket of another protein kinase may be readily determined by one skilled in the art. For example, when the protein kinase is selected from a protein listed in Table 1, the root mean square deviation is preferably within about 2.7 angstroms, and is more preferably within about 2.5 angstroms.

This invention also provides a method for identifying a potential agonist or antagonist of a molecule comprising a P38γ-like binding pocket, comprising the steps of:

a) creating a computer model of the binding pocket using structure coordinates wherein:

(i) the root mean square deviation between said structure coordinates and the structure coordinates of the P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1 is within about 3.0 angstroms,

(ii) said binding pocket model depicts amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, and

(iii) said binding pocket model depicts the ψ angle of the residue corresponding to Met112 to be in the range of about -60° to 60° and the ϕ angle of the residue

corresponding to Gly113 to be in the range of about 30° to 150°;

b) employing said model of the binding pocket to design or select said potential agonist or antagonist;

c) synthesizing said agonist or antagonist; and

d) contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

A preferred embodiment of this method uses the structure coordinates of the Met112 and Gly113 amino acids of p38γ or the Met112 and Gly113 equivalent residues of a protein listed in Table 1.

In order that this invention be more fully understood, the following examples are set forth. These examples are for the purpose of illustration only and are not to be construed as limiting the scope of the invention in any way.

Example 1

Expression and Purification of P38γ Protein

P38 with a His6 tag was overexpressed in *E.Coli*, and then purified by using metal affinity resin followed by MonoQ resin. The purified material was phosphorylated with constituitively active MKK6, and purified again with MonoQ resin (Fox, T. et al., manuscript in preparation). Size-exclusion chromatography was performed to determine the apparent molecular weights of unphosphorylated and phosphorylated P38γ as follows. A Superdex 75 HR 10/30 column (Pharmacia, Uppsala) was equilibrated in 12.5 mM HEPES, pH 7.3, containing 6.25 % (v/v) glycerol and 100 mM KCl. Bovine serum albumin (67 kDa), ovalbumin (43 kDa), chymotrypsinogen (25 kDa), ribonuclease A (13.7 -

kDa) were used to calibrate the column prior to P38γ analyses. A flow rate of 0.25 ml/min was used for chromatographic runs and samples were loaded in a volume of 100-200 _l at 0.7 - 4 mg/ml.

Example 2

Crystallization of P38γ

Crystals of phosphorylated P38γ complexed with AMP-PNP were grown by vapor diffusion. Clusters of rods appeared after 3 to 7 days when protein (0.5 mM P38γ with 5 mM AMP-PNP and 0.02% $C_{12}E_9$) was mixed with an equal volume of reservoir (100 mM NaOAc, 100 mM Tris 8.5, 27% PEG 4000, 10 mM $MgCl_2$, and 5 mM DTT) and allowed to stand at room temperature. Single crystals with 100 mM maximum thickness were separated from their parent cluster, cryoprotected by adding ethylene glycol to a final concentration of 15% over 15 min in three equal steps, and flash cooled to -170°C in a stream of gaseous nitrogen.

Example 3

X-Ray Data Collection and Structure Determination

The diffraction pattern displayed symmetry consistent with space group $P2_12_12_1$, with unit cell dimensions a=63.50Å, b=66.82Å, and c=206.02Å. Diffraction extended to 4.0Å in the a*, b* direction and 3.0Å in the c* direction. Data collection at NSLS X25 allowed a significant improvement in the observed diffraction limit: data were collected to 3.0Å in the a*,b* direction and at least 2.4Å in the c* direction. Data were integrated to 2.4Å [Otwinowski, Z. in *CCP4 Study Weekend* (eds. Sawyer, L., Isaacs, N. & Bailey, S.) 56-62 (SERC

Daresbury Laboratory, England) (1993); Minor, W. XDISPLAYF Program, Purdue University, (1993)]. The overall R-merge for the data was 6.7%, with I/sig(I)=2.0 at 2.4Å resolution. The X-ray data comprised 31732 unique reflections derived from 118429 intensity measurements. The data were 90% complete overall and 76.5% complete in the 2.49-2.40Å resolution shell. Data incompleteness, particularly in the highest resolution shell, reflects the anisotropic nature of the diffraction.

The volume of the asymmetric unit indicated the presence of two P38γ molecules. The self-rotation function calculated with POLARRFN [*Acta Crys* D50, 760-763 (1994)] revealed a noncrystallographic peak with intensity half of the origin at Kappa =180°, omega=90°, and Phi=44°.

Coordinates for the structure of phosphorylated ERK2 were not initially available from the protein data bank and could not be used for molecular replacement. Several different models for P38γ were constructed based on the X-ray coordinates of P38γ or unphosphorylated ERK2 with either all side chains truncated to alanine, or with only the nonconserved side chains truncated to alanine or glycine [Zhang et al., *Nature* 367, 704-711 (1994); Wilson and Su, *J Biol Chem* 271, 27696-27700 (1996)]. No rotation function solutions were obtained using these models with either the X-plor or AMORE molecular replacement packages. The anisotropy of the data, as well as the presence of two molecules in the asymmetric unit, could be reasons for the lack of a successful molecular replacement solution. Variability in the orientation between the large and small kinase domains may have been an additional complicating factor.

To position correctly an initial P38γ model, experimental phases at low resolution were obtained from two derivatives. Crystals were soaked with 0.2 mM ethylmercurychloride (EMP) for 5 days, and with 2 mM $EuCl_3$ overnight. Diffraction data were collected on the in house RaxisIIc, and integrated to 5.0Å [see Owinowski and Minor, supra]. Difference Patterson maps were interpreted by using SHELXS-97 [*Acta Crys* **A46**, 467-473 (1990)]. The EMP derivative yielded four sites and the Europium derivative yielded two sites. These heavy atom positions were refined by using ML-PHARE [*Acta Crys* **D50**, 760-763 (1994)] which yielded an overall figure of merit of 0.53 to 5Å. The resulting electron density maps showed clear solvent and protein regions. Six heavy atom sites were identified within a continuous envelope of protein density and grouped into two sets of three sites. These two sets were related to one another by a two-fold axis, which was consistent with the self-rotation function. Each set of three sites was assumed to correspond to a monomer of P38γ, and the two-fold operation was used to improve the experimental electron density by noncrystallographic symmetry (NCS) averaging. Solvent flattening combined with two-fold averaging using Dm (final correlation coefficient of averaging of 0.851) produced an electron density map at 5.0Å that allowed placement of the P38γ model. The N-terminal domain had to be rotated by several degrees with respect to the C-terminal domain in order to fit both domains into the experimental density. At this stage the model was refined against the high resolution synchrotron data. Rigid body refinement and torsional dynamics refinement yielded an initial R_{free} of 42%.

The quality of the model was improved by cycles of

model building, positional refinement, and thermal factor refinement, interspersed with torsional dynamics runs using data from 50.0 to 2.4Å. All stages of model refinement were carried out using the new program CNS [*Acta Crys* D54, 905-921 (1988)] with bulk solvent correction and anisotropic scaling. NCS restraints were applied throughout the refinement. The current P38γ model contains two monomers, each with 329 protein residues, one bound AMP-PNP molecule, and two Mg^{2+} ions. A total of 186 water molecules were included in the entire asymmetric unit. The current R_{work} is 23.2% (R_{free} = 28.3%) versus all data with |F| > 2_(F) between 50-2.4Å resolution (27841 reflections). PROCHECK was used to analyze the model stereochemistry [*Acta Crys* D50, 760-763 (1994)]. All of the residues were in the most favored and additional allowed regions of the Ramachandran plot. One residue per monomer (Val187) from the phosphorylation loop was in the disallowed region. The P38γ model has deviations from ideal bond lengths and angles of 0.010Å and 1.63° respectively. No electron density was observed for amino acids 1-7, 34-39, 316-321, 330-334, and 354-end, therefore these residues were not included in the model. The eight residue histidine tag and 21 residues at the C-terminus are also disordered. Subsequent to the structure refinement, the phosphorylated ERK2 coordinates were released, and the final refined P38γ structure was compared with that structure.

Example 4

Overall Structure

The P38γ structure was solved with a combination of low resolution MIR and molecular replacement using a

model of the unphosphorylated form of P38α [Wilson and Su, *J Biol Chem* 271, 27696-27700 (1996)]. The current structure includes two P38γ molecules per asymmetric unit, each with 329 amino acids, a bound AMP-PNP, and two Mg^{2+} ions. A total of 186 water molecules were modeled in the asymmetric unit. The current R_{free} and R_{work} are 28.3% and 23.2%, respectively. The refined model has deviations from ideal bond lengths and angles of 0.01Å and 1.6°. The two P38γ molecules in the asymmetric unit superimpose with an overall r.m.s.d. of 0.013Å using all Cα atoms, and thus represent two independent but highly similar structures of activated P38γ.

Comparison of Kinase Structures

Electron density for the main chain atoms of P38γ is visible from residue 8 to 353, with breaks at residues 34-39, 316-321 and 330-334 (Fig. 1). The glycine rich loop, which contains the consensus Gly-X-Gly-X-X-Gly sequence (residues 34-39 in P38γ) is mobile, and residues 34-39 could not be modeled. The homologous region of P38α is also flexible, and has average B-values equal to 61Å. In contrast, the AMP-PNP ligand is well ordered, as are all nearby secondary structural elements. Strong electron density for the residues at the N- and C-terminal ends of the glycine rich loop is also observed. The C-terminal 40 residues of both P38γ molecules in the asymmetric unit are not as well ordered as the rest of the structure. Helix αL16 can be modeled, but contains several disordered side chains. The region just before helix αL16 is poorly ordered and does not form the 3/10 helix L16 observed in the structure of phosphorylated ERK2. Helix αL16 and 3/10 helix L16 are involved in

dimer formation in the structure of phosphorylated ERK2 [Canagarajah et al., *Cell* 90, 859-869 (1997)].

Activated P38γ contains a small amino terminal domain comprised mainly of β-strands, and a large carboxyl terminal domain that consists mostly of α-helices (Fig. 1). This fold is common among kinases [Taylor & Radzio-Andzlem (1994); *Structure* 2, 345-355; Kultz *J Mol Evol* 46, 571-588 (1998)]. A deep cleft at the interface between the domains forms the binding site for ATP and Mg^{2+}. The two domains are connected by a hinge, located at a point adjacent to the adenine base and near residue 113 (Fig. 1).

Whereas the sequence, fold, and topology of P38γ is similar to P38α (Figs. 1, 2), the domains of activated P38γ are closed relative to P38α Independent superimpositions of the domains of P38γ onto the P38α structure yield r.m.s. deviations of 1.2Å for the N-terminal domain (P38γ Cα carbons from residues 10-16, 19-33, and 40-113), and 0.62Å for the C-terminal domain (P38γ C_α carbons from residues 125 to 160, 206 to 238 and 282 to 297). Greater differences between P38γ and P38α are observed when the whole proteins are compared. Superimposition of the C-terminal domain of P38γ onto the corresponding lobe of P38α revealed a rotation of the N-terminal domain of P38γ by 20° relative to the orientation seen in P38α (Fig. 2). Other differences between the structure of phosphorylated P38γ and P38α occur in the conformation of α1L14, α2L14, α1L12, the phosphorylation loop, and αL16.

Inter-domain rotation, or domain closure, is common in MAP kinase structures, and is observed to different extents. The structures of unphosphorylated and phosphorylated ERK2 show a 5° difference in domain

closure. The structure of unphosphorylated JNK3 reveals that a 10° domain rotation would be needed to superimpose both domains with the structure of phosphorylated P38γ or phosphorylated ERK2. P38α MAP kinase is more open in its unphosphorylated state than ERK2 or JNK3. Despite a large difference in the conformations of the unphosphorylated proteins, the domains of the activated forms of P38γ and ERK2 can be superimposed with a rotation of only 3°. Comparison to solved kinase structures indicates that the relative positions of the domains in activated P38γ is most similar to activated ERK2 MAP kinase.

The structures of phosphorylated P38γ and phosphorylated ERK2 are similar, with a few significant differences. One conformational difference is a movement of the α1L14, α2L14 helical region. With the large domains superimposed, the difference in α1L14, α2L14 orientation between the two structures is about 6Å, when measured at the most extreme portion of the helices. Another difference between the two structures is that the P38γ activation loop is six residues shorter than the activation loop in ERK2. Excluding these two regions allows one to superimpose P38γ Cα carbons 19-33, 40-58, 61-94, 97-113, 117-177, 182-243, and 269-315 with the corresponding ERK2-P2 atoms to yield an r.m.s.d. of 1.1Å. This reflects the high similarity between the two structures. A comparison of the activation loops, using P38γ Cα carbons 173-177 and 182-188 yields an r.m.s.d. of 0.3Å.

The structure of the phosphorylation loop differs between phosphorylated P38γ and unphosphorylated P38α (Fig. 2). The phosphorylation loop contains the TGY sequence present in all P38 MAP kinases. Phosphorylation

of Thr183 and Tyr185 results in a movement of the activation loop, and produces changes in the P38γ structure.

Phospho-Thr183 sits at the interface between the two domains. The Thr183 phosphate group interacts with Arg70, Arg73 and Lys69 from the N-terminal domain, and Arg152 and Arg176 from the C-terminal domain (Figs. 1 and 3). The two domains are connected by a hinge, located at a point adjacent to the adenine base and near residue 113. The hinge-point and residue pThr183 are located at opposite ends of the interface between the two domains. The network of interactions between pThr183 and these basic residues pulls the domains together. As a result, the relative orientations of the amino acids, including the catalytic residues, located between the hinge and pThr183 are changed. A similar set of interactions between the phospho-threonine and nearby basic residues was reported for the structure of phosphorylated ERK2 [Canagarajah et al., *Cell* 90, 859-869 (1997)]. Phosphorylated P38γ is in a conformation consistent with activity. The active site of phosphorylated P38γ is shown in detail in Fig. 4, and compared with the active sites of P38α and cAPK in Figs, 5a and 5b. The interactions between the non-hydrolyzable nucleotide analog AMP-PNP and P38γ (Fig. 4) are very similar to those made between bound nucleotide and cAPK [Zheng et al.,*Acta Cryst.* D49, 362-365 (1993); Bossemeyer et al., *EMBO Journal* 12, 849-859 (1993); Narayana et al., *Structure* 5, 921-935 (1997)].

The N1 and N6 nitrogen atoms of AMP-PNP form hydrogen bonds to the backbone amide nitrogen atom of Met112 and the backbone carbonyl oxygen atom of Pro110, respectively. Interactions between the glycine rich loop and the nucleotide

are not observed in the P38γ structure.

The relative positions of catalytic residues Lys53, Glu74 and Asp153 provide information about the state of activation of the kinase [Kumar et al., *J. Biol. Chem.* 270, 29043-29046 (1995); Robinson et al., *Curr Opin Cell Biol* 9, 180-186 (1997)]. Comparison of P38γ with cAPK after superimposing the nucleotides from the two structures (Fig. 5b), reveals that the active site residues in the two structures are in almost the same conformation. The cAPK structure also contains a bound peptide inhibitor, and the complex is believed to represent a bioactive conformation of cAPK [Zheng et al, supra; Bossemyer et al., supra; Narayana et al., supra]. The nucleotides in both structures adopt almost the same conformations, and the relative positions of the catalytic residues Lys-56, Glu-74 and Asp-153 are conserved. There are also two bound metal ions in each complex. After superimposition, metal I in cAPK is separated from the corresponding metal in P38α by 0.5Å, and metal II from P38γ is 1.4Å removed from metal II in cAPK. Because the conformation and relative orientation of the catalytic residues and cofactors in the active sites of the two kinases are almost the same, the structure of phosphorylated P38γ described here is likely to represent an active conformation.

Comparing the phosphorylated P38γ to the known, unphosphorylated P38α one finds that the active site residues of P38α are significantly displaced relative to their orientation in P38γ. This presumably reflects the inactive state of unphosphorylated P38α (Fig. 5a). Two types of structural differences are observed between unactivated P38α and activated P38γ. A rigid body motion occurs between the two domains, and secondary structure

elements and residues move as a result of phosphorylation and AMP-PNP binding.

Using the newly-determined structure of P38γ, the structure of unphosphorylated P38α could be altered to properly position its catalytic residues in an active conformation. Without the P38γ structural information, it was not known whether domain movement alone would be enough to properly position the catalytic residues in an active conformation or whether activation would also require other changes [Johnson et al., *Curr. Opin. Struct. Biol.* **6**, 762-769 (1996); Yamaguchi et al., *Nature* 384, 484-489 (1996); Johnson et al., *Cell* 85, 149-158 (1996); Russo et al., *Nature Struc Biol* 3, 696-700 (1996)].

To address this question, the structure of unphosphorylated P38α was altered to resemble phosphorylated P38γ. Only a rigid-body movement, centered on the hinge residue 113, was used to change the relative orientation of the two domains in P38α. The resulting model maintains the detailed secondary structure features present in non-phosphorylated P38α, but has the same domain closure as P38γ. The positions of catalytic residues in the active site of this modified P38γ model match well to those observed in the structure of activated P38γ. The rigid body movement shifts P38α residue Lys-53 2.9Å closer to its counterpart in P38γ(from 4.4Å to 1.5Å separation). Glu-71 (P38α) moves 2.8Å nearer to its equivalent residue in P38γ(from 3.2Å to 0.4Å separation). Thus, the structures of P38α and P38γ suggest that a simple domain rotation accounts for most of the rearrangement of catalytic residues necessary for activation of P38γ.

Other movements may contribute to activation of P38γ.

For example, phosphorylation of Tyr185 leads to a rearrangement of surrounding secondary structure elements that may effect substrate binding. Arg192 interacts with the pTyr185 phosphate group in the P38γ structure, and is shifted more than 5Å relative to its position in the apo-P38α structure. Such coordination of Arg 192 and its effect on substrate binding have been discussed with regard to ERK2 and JKN3 [Zhang, *Nature* 367, 704-711 (1994); Xie and Su, supra; Canagarajah, supra]. In the P38γ structure, pTyr185 interacts directly with Arg189 and Arg192 (Fig. 3). Comparison of the P38γ pTyr185 conformation, as well as the backbone conformation with the corresponding residue of phosphorylated ERK2, shows that the two residues are in nearly the same conformation.

Activated P38_ is Monomeric

The two P38γ proteins in the crystallized complex show no evidence of dimeric interaction, as evidenced by the examination of the activation loops of the two proteins. This is unlike the activated, phosphorylated ERK2, which is believed to reveal a dimer interface that is not observed in the non-phosphorylated form [Zhang et al., supra; Canagarajah et al., supra; Khokhlatchev et al., supra]. The dimer interface in phosphorylated ERK2 reportedly buries a total of 1470Å^2 of surface area, and is formed in part by an ion pair between His176 from one molecule and Glu343 from the other molecule. In addition, Leu333, Leu336, and Leu344 are reported to further stabilize the dimer interface.

The entire surface of each P38γ molecule in the asymmetric unit was examined in search of any dimer interface. The crystal of P38γ belongs to space group

$P2_12_12_1$, which contains only two-fold screw axes, but no crystallographic two-fold axes. The only two-fold axis in the crystal is the non-crystallographic axis which relates the two molecules within the asymmetric unit. This dimeric interaction involves Pro282, Asn286, Lys290, Leu283, Pro309, and Glu312. This non-crystallographic dimer interface buries only 680Å^2 of surface area, less than half of the 1470Å^2 buried in the phosphorylated ERK2 dimer interface.

To characterize further the oligomeric state of activated P38γ in solution, size-exclusion chromatography was performed to determine the apparent molecular weights of unphosphorylated and phosphorylated P38γ. To facilitate comparison with the phosphorylated ERK2 results [Khokhlatchev et al., supra], the same column resin, buffer, and loading conditions were used. The chromatographic profiles of unphosphorylated and phosphorylated P38γ showed that both proteins eluted with a similar retention time, corresponding to a molecular weight of 44.5 kDa as determined from the protein calibration curve. The absence of dimer formation of phosphorylated P38γ in solution is consistent with the absence of dimer formation in the crystal structure of P38γ. It is also consistent with the absence of dimer formation in ERK2 mutants where His176 is deleted [Khokhlatchev et al., supra].

Conformations of Activation Loops of Kinases

The number of residues in the activation loops of different kinases varies, ranging from 8 amino acids in calmodulin dependent DAP-kinase to 37 residues in LIMK2 [Deiss et al., *Genes Dev.* 9, 15-30 (1995); Okano et al., *J. Biol. Chem.* 270, 31321-31330 (1995)]. The P38γ

activation loop consists of residues Gly173-Thr188. The phosphorylation loop of ERK2 is six residues longer in sequence and spans amino acids Gly167-Thr188. The loop region of cAPK is the same length as P38γ, and spans amino acids Gly186-Thr201. Fig. 6 highlights the loop regions from P38γ, ERK2-P2, and cAPK. Except for a longer loop size for ERK2, the structures of the loop regions of activated P38γ and activated ERK2 are nearly identical. The distance between the phosphate moieties from Thr183 in P38γ and ERK2 is only 0.4Å, and separation between the Tyr185 phosphate from P38γ and ERK2 is 1.6Å. The phosphorylation loop of cAPK does not superimpose as well with the two MAP kinase phosphorylation loops, although the Thr phosphate is only 2.0Å away from the P38γ Thr183 phosphate. The phosphorylation loop regions from P38γ, ERK2 and cAPK have different lengths, but in their phosphorylated states adopt almost the same conformations.

Figures 1a-6 further depict the structure of the phosphorylated P38γ/MgAMP-PNP complex. Thus, Fig 1a depicts an overview of the phosphorylated P38γ structure. The large and small domains are pulled together by interactions mediated by phospho-Thr183. Ribbon diagrams of the activated P38γ structure with the amino-terminal small domain are colored light orange and the carboxy-terminal large domain colored blue. The interface between the two domains (residue 113) can be thought of as a hinge point through which domain movement occurs. Four Arg residues and one Lys residue are explicitly shown coordinated to the phosphate of pThr183. Arg70, Arg73 and Lys69 anchor the small domain to pThr183, and Arg152 and Arg176 anchor the large domain to pThr183. PThr183 pulls the domains together. All figures were

made with RIBBONS [Carson et al., *J. Mol. Graphics* **4**, 121-122 (1986)].

Fig 2 is a superimposition of the structures of unphosphorylated P38α and phosphorylated P38γ. P38α is shown in light blue and dark blue (activation loop), and P38γ is shown in light orange and dark orange (activation loop). The Cα atoms from residues 125 to 160, 206 to 238 and 282 to 297 were used to superimpose the two proteins with an r.m.s.d. of 0.62Å. Also shown is the AMP-PNP and two Mg^{2+} ions from the P38γ structure. All atoms of the phosphorylated Thr183 and Tyr185 from the P38γ structure are shown. Major changes upon phosphorylation are a significant domain closure and a rearrangement of the activation loop.

Fig 3 is a detailed stereo view of activation loop. All atom stereo view of the P38γ activation loop (residues 174 to 189). Residues that coordinate pThr183 and pTyr185 are also shown. Hydrogen bonds are indicated with dashed grey lines. The phosphate atoms are shown in pink.

Fig 4 is a stereo view of AMP-PNP. All major interactions with protein sidechains are indicated with dashed grey lines. The bound Mg^{2+} ions are indicated by black spheres. The phosphate atoms are shown in pink. Met109 can be seen behind the adenine base, blocking the hydrophobic pocket. Water molecules have been removed for clarity.

Figures 5a and 5b are a comparison of the active site of activated P38γ with P38α and cAPK. P38γ is shown in orange, P38α in blue, and cAPK in red. In all three structures a salt bridge is observed between Lys56 and Glu74 (P38γ numbering). a) Comparison of the active

sites of P38γ with P38α by superimposition of their carboxyl terminal large domains. Catalytic residues are misaligned. The distance between Asp153 and Lys53 is 12.6Å in the P38α structure compared with 8.5Å in the phosphorylated P38γ structure. b) Comparison of the active sites of P38γ with cAPK (Protein Data Base code: 1ATP, ref. 22) by superimposition of all atoms of their bound AMP-PNP molecules. All catalytic residues align to within a fraction of an Å. The distance between Asp153 and Lys53 is 8.5Å in the activated P38γ structure. This distance is very close to the distance of 7.8Å observed in activated cAPK, suggesting that the structure reported here is of the activated kinase. Asp171 is excluded from these figures for clarity because it is obscured by AMP-PNP and Mg^{2+} ions.

Fig 6 is a comparison of activated phosphorylation loops from P38γ (dark orange), ERK2 (dark blue), and cAPK (red). Superimposition of these three structures was with the C_α atoms of residues 125 to 160, 206 to 238 and 282 to 297 of P38γ. In order to ensure an unbiased comparison of the lip regions, these residues were omitted from the calculation. All three lip regions have different lengths, but have surprisingly similar conformation. Comparison of P38γ and ERK2 superimposes the two phorphorylated amino acids almost exactly, despite a six amino acid difference in length. The phosphorylated Thr197 of cAPK also superimposes well with the two MAP kinase structures. This comparison suggests that the phosphorylated lip structures observed in P38γ and ERK2 may be representative of all MAP kinases.

Example 5

The Use of P38γ/MgAMP-PNP
Coordinates for Inhibitor Design

The coordinates of Figure 1 are used to design compounds, including inhibitory compounds, that associate with P38γ or homologues of P38γ. This process may be aided by using a computer comprising a machine-readable data storage medium encoded with a set of machine-executable instructions, wherein the recorded instructions are capable of displaying a three-dimensional representation of the P38γ/MGAMP-PNP complex or a portion thereof. The graphical representation is used according to the methods described herein to design compounds. Such compounds associate with the P38γ at the active site.

Example 6

P38γ Activity Inhibition Assay

To determine the IC_{50} of compound binding to P38γ, the kinase activity of P38Y was monitored by coupled enzyme assay. In this assay, for every molecule of ADP generated by the P38Y kinase activity one molecule of NADH is converted to NAD which can be conveniently monitored as an absorbance decrease at 340 nm. The following are the final concentrations of various reagents used in the assay: 100 mM HEPES buffer, pH 7.6, 10 mM $MgCl_2$, 30 μM ATP, 2 mM phosphoenolpyruvate, 2 μM pyruvate kinase, 2 μM lactate dehydrogenase, 200 μM NADH, 200 μM EGF receptor peptide KRELVEPLTPSGEAPNQALLR, and 10 nM activated P38γ. First, all of the above reagents with

the exception of ATP were mixed and 175 µl aliquots were placed per well of 96-well plate. A 5 µl DMSO solution of the compound was added to each well, mixed, and allowed to stand at 30°C for 10 minutes. Typically about 10 different concentrations of the compound were tested. The reactions were initiated with the addition of 20 µl of ATP solution. Absorbance change at 340 nm were monitored as a function of time. IC_{50} is obtained by fitting the rates vs. compound concentration data to a simple competitive inhibition model.

While we have described a number of embodiments of this invention, it is apparent that our basic constructions may be altered to provide other embodiments which utilize the products, processes and methods of this invention. Therefore, it will be appreciated that the scope of this invention is to be defined by the appended claims, rather than by the specific embodiments which have been presented by way of example.

We claim:

1. A crystalline composition comprising a phosphorylated P38 protein-ligand complex.

2. The crystalline composition of claim 1 wherein the complex is capable of being resolved at 2.4A resolution, the complex comprising:

a) a purified enzyme selected from phosphorylated P38α, phosphorylated P38β, phosphorylated P38δ, phosphorylated P38γ, or a phosphorylated isoform of any of the foregoing;

b) a ligand; and

c) magnesium ions.

3. The crystalline composition according to claim 2, wherein said enzyme is P38γ.

4. A crystalline protein kinase-ligand complex, said kinase comprising a binding pocket defined by the structure coordinates of the P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1, or a homologue of said kinase, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å.

5. A crystalline protein kinase-ligand complex, said

kinase selected from the proteins listed in Table 1, wherein the ψ angle of the residue corresponding to Met112 of p38γ is in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 of p38γ is in the range of about 30° to 150°.

6. A crystalline protein kinase-ligand complex, said kinase comprising amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, wherein the ψ angle of the residue corresponding to Met112 is in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 is in the range of about 30° to 150°.

7. A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex comprising a binding pocket, said method comprising the steps of:

a) creating a computer model of the binding pocket using structure coordinates wherein the root mean square deviation between said structure coordinates and the structure coordinates of the P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1 is not more than about 1.15 Å;

b) employing computational means to perform a fitting operation between the chemical entity and said

computer model of the binding pocket; and

c) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket model.

8. The method according to claim 7, wherein said binding pocket is further defined by the structure coordinates of P38γ amino acids Pro32, Cys42, Ser43, Val53, Ilè55, Lys57, Leu58, Thr59, Arg70, Glu74, Gly88, Leu107, Val108, Leu116, Gly117, Pro156, Leu159, Val161, Lys168, Phe172, Ala175, and Thr188 according to Figure 1.

9. The method according to claim 8 wherein said molecule or molecular complex is defined by the set of structure coordinates for all P38γ amino acids according to Figure 1.

10. A method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure, comprising the steps of:

a. crystallizing said molecule or molecular complex;

b. generating an X-ray diffraction pattern from said crystallized molecule or molecular complex;

c. applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

11. A computer for producing a three-dimensional representation of a molecule or molecular complex,

wherein said computer comprises:

a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said machine-readable data comprises the structure coordinates of P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1, or structural coordinates having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å;

b) a working memory for storing instructions for processing said machine-readable data;

c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium, for processing said machine readable data into said three-dimensional representation; and

d) an output hardware coupled to said central-processing unit, for receiving said three-dimensional representation.

12. A method for identifying a potential agonist or antagonist of a molecule comprising a P38γ-like binding pocket, comprising the steps of:

a. using the atomic coordinates of Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å, to generate a three-dimensional structure of molecule comprising the P38γ-like binding pocket;

b. employing said three-dimensional structure to design or select said potential agonist or antagonist;

c. synthesizing said agonist or antagonist; and

d. contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

13. The method according to claim 12, wherein the atomic coordinates of Pro32, Val33, Ala40, Val41, Cys42, Ser43, Val53, Ala54, Ile55, Lys56, Lys57, Leu58, Thr59, Arg70, Glu74, Ile87, Gly88, Leu107, Val108, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Leu116, Gly117, Lys118, Asp153, Lys155, Pro156, Gly157, Asn158, Leu159, Ala160, Val161, Lys168, Leu170, Asp171, Phe172, Gly173, Leu174, Ala175, and Thr188 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å, are used to generate said three-dimensional structure of the molecule comprising a P38γ-like binding pocket.

14. The method according to claim 13, wherein the atomic coordinates of all the amino acids of P38γ according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å, are used to generate a three-dimensional structure of molecule comprising a P38γ-like binding pocket.

15. A computer for producing a three-dimensional representation of a protein kinase or a protein kinase-ligand complex, or portion thereof, wherein said computer comprises:

a) a machine-readable data storage medium comprising

a data storage material encoded with machine-readable data, wherein said machine-readable data comprises the structure coordinates of said kinase, or portion thereof, said kinase or portion thereof comprising amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, wherein the ψ angle of the residue corresponding to Met112 is in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 is in the range of about 30° to 150°;

b) a working memory for storing instructions for processing said machine-readable data;

c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium, for processing said machine readable data into said three-dimensional representation; and

d) an output hardware coupled to said central-processing unit, for receiving said three-dimensional representation.

16. A method for evaluating the ability of a chemical entity to associate with a protein kinase binding pocket, said method comprising the steps of:

a) creating a computer model of the binding pocket using structure coordinates wherein:

(i) the root mean square deviation between said structure coordinates and the structure coordinates of the P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160,

Leu170, Asp171, Gly173, and Leu174 according to Figure 1 is within about 3.0 angstroms,

(ii) said binding pocket model depicts amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, and

(iii) said binding pocket model depicts the ψ angle of the residue corresponding to Met112 to be in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 to be in the range of about 30° to 150°;

b) employing computational means to perform a fitting operation between the chemical entity and the binding pocket model; and

c) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket model.

17. A method for identifying a potential agonist or antagonist of a molecule comprising a P38γ-like binding pocket, comprising the steps of:

a) creating a computer model of the binding pocket using structure coordinates wherein:

(i) the root mean square deviation between said structure coordinates and the structure coordinates of the P38γ amino acids Val33, Ala40, Val41, Ala54, Lys56, Ile87, Met109, Pro110, Phe111, Met112, Gly113, Thr114, Asp115, Lys118, Asp153, Lys155, Gly157, Asn158, Ala160, Leu170, Asp171, Gly173, and Leu174 according to Figure 1 is within about 3.0 angstroms,

(ii) said binding pocket model depicts amino acid residues that correspond by functional and/or sequence alignment to the Met112 and Gly113 residues of P38γ or that correspond by functional and/or sequence alignment to the Met112 and Gly113 equivalent residues of one or more proteins listed in Table 1, and

(iii) said binding pocket model depicts the ψ angle of the residue corresponding to Met112 to be in the range of about -60° to 60° and the ϕ angle of the residue corresponding to Gly113 to be in the range of about 30° to 150°;

b) employing said model of the binding pocket to design or select said potential agonist or antagonist;

c) synthesizing said agonist or antagonist; and

d) contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1	N	ARG	A	8	50.744	68.953	-19.867	1	82.26
2	CA	ARG	A	8	51.733	70.011	-19.529	1	82.91
3	C	ARG	A	8	52.844	69.485	-18.592	1	83.38
4	O	ARG	A	8	52.777	68.355	-18.091	1	83.08
5	CB	ARG	A	8	51.013	71.214	-18.918	1	80.87
6	N	SER	A	9	53.885	70.296	-18.408	1	83.59
7	CA	SER	A	9	55.028	69.954	-17.564	1	82.36
8	C	SER	A	9	55.82	71.228	-17.264	1	80.92
9	O	SER	A	9	55.748	72.203	-18.014	1	79.73
10	CB	SER	A	9	55.931	68.93	-18.27	1	85.39
11	OG	SER	A	9	56.938	68.428	-17.399	1	87.48
12	N	GLY	A	10	56.597	71.198	-16.181	1	80.75
13	CA	GLY	A	10	57.381	72.357	-15.774	1	77.56
14	C	GLY	A	10	56.625	73.137	-14.711	1	75.22
15	O	GLY	A	10	55.874	72.55	-13.928	1	74.7
16	N	PHE	A	11	56.834	74.45	-14.659	1	72.75
17	CA	PHE	A	11	56.147	75.305	-13.687	1	68.57
18	C	PHE	A	11	55.637	76.563	-14.371	1	69.71
19	O	PHE	A	11	55.787	76.723	-15.583	1	70.87
20	CB	PHE	A	11	57.072	75.702	-12.532	1	63.69
21	CG	PHE	A	11	57.413	74.576	-11.61	1	60.38
22	CD1	PHE	A	11	58.404	73.649	-11.952	1	62.55
23	CD2	PHE	A	11	56.744	74.425	-10.402	1	60.69
24	CE1	PHE	A	11	58.724	72.575	-11.097	1	62.34
25	CE2	PHE	A	11	57.054	73.352	-9.535	1	63.35
26	CZ	PHE	A	11	58.047	72.427	-9.886	1	60.96
27	N	TYR	A	12	54.981	77.421	-13.597	1	70.53
28	CA	TYR	A	12	54.466	78.687	-14.098	1	73.77
29	C	TYR	A	12	54.029	79.569	-12.935	1	75.91
30	O	TYR	A	12	53.839	79.088	-11.817	1	76.32
31	CB	TYR	A	12	53.378	78.485	-15.165	1	74.03
32	CG	TYR	A	12	51.952	78.365	-14.693	1	77.25
33	CD1	TYR	A	12	51.387	77.116	-14.424	1	76.91
34	CD2	TYR	A	12	51.13	79.494	-14.611	1	78.07
35	CE1	TYR	A	12	50.036	76.99	-14.094	1	78
36	CE2	TYR	A	12	49.778	79.38	-14.279	1	79.84
37	CZ	TYR	A	12	49.237	78.123	-14.027	1	79.01
38	OH	TYR	A	12	47.896	77.997	-13.743	1	80.18
39	N	ARG	A	13	53.909	80.867	-13.187	1	78.58
40	CA	ARG	A	13	53.571	81.807	-12.124	1	81.99
41	C	ARG	A	13	52.314	82.607	-12.411	1	82.41
42	O	ARG	A	13	52.003	82.886	-13.565	1	82.24
43	CB	ARG	A	13	54.769	82.74	-11.896	1	85.09
44	CG	ARG	A	13	56.127	81.98	-11.974	1	91.35
45	CD	ARG	A	13	57.415	82.803	-11.776	1	95.98
46	NE	ARG	A	13	57.109	83.991	-11.068	1	99.39
47	CZ	ARG	A	13	57.291	84.52	-9.871	1	100
48	NH1	ARG	A	13	57.95	84.023	-8.831	1	100
49	NH2	ARG	A	13	56.578	85.628	-9.741	1	99.54
50	N	GLN	A	14	51.6	82.986	-11.354	1	83.93
51	CA	GLN	A	14	50.377	83.763	-11.509	1	85.5
52	C	GLN	A	14	50.056	84.671	-10.332	1	86.86
53	O	GLN	A	14	50.422	84.392	-9.191	1	85.56
54	CB	GLN	A	14	49.187	82.834	-11.751	1	86.15
55	CG	GLN	A	14	47.917	83.565	-12.165	1	86.97
56	CD	GLN	A	14	46.734	82.636	-12.364	1	87.55

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
57	OE1	GLN	A	14	45.605	82.969	-11.987	1	86.77
58	NE2	GLN	A	14	46.979	81.473	-12.966	1	87.48
59	N	GLU	A	15	49.405	85.785	-10.651	1	90.02
60	CA	GLU	A	15	48.971	86.764	-9.667	1	94
61	C	GLU	A	15	47.613	86.293	-9.182	1	96.77
62	O	GLU	A	15	46.654	86.27	-9.958	1	98.74
63	CB	GLU	A	15	48.793	88.135	-10.328	1	95.34
64	CG	GLU	A	15	48.068	88.087	-11.686	1	99.57
65	CD	GLU	A	15	47.489	89.436	-12.131	1	100
66	OE1	GLU	A	15	48.282	90.349	-12.468	1	100
67	OE2	GLU	A	15	46.24	89.564	-12.173	1	100
68	N	VAL	A	16	47.523	85.869	-7.927	1	98.29
69	CA	VAL	A	16	46.234	85.43	-7.414	1	99.04
70	C	VAL	A	16	45.526	86.621	-6.758	1	100
71	O	VAL	A	16	44.777	87.347	-7.429	1	100
72	CB	VAL	A	16	46.382	84.225	-6.476	1	99.49
73	CG1	VAL	A	16	45.022	83.812	-5.929	1	100
74	CG2	VAL	A	16	46.965	83.07	-7.261	1	98.21
75	N	THR	A	17	45.718	86.811	-5.457	1	98.92
76	CA	THR	A	17	45.114	87.969	-4.809	1	99.7
77	C	THR	A	17	46.237	88.998	-4.8	1	100
78	O	THR	A	17	46.526	89.626	-5.83	1	100
79	CB	THR	A	17	44.62	87.671	-3.38	1	99.48
80	OG1	THR	A	17	45.267	86.493	-2.879	1	100
81	CG2	THR	A	17	43.094	87.496	-3.367	1	97.76
82	N	LYS	A	18	46.915	89.11	-3.663	1	100
83	CA	LYS	A	18	48.037	90.027	-3.534	1	99.44
84	C	LYS	A	18	49.334	89.23	-3.691	1	98.74
85	O	LYS	A	18	50.377	89.783	-4.052	1	99.4
86	CB	LYS	A	18	47.997	90.713	-2.167	1	99.64
87	N	THR	A	19	49.233	87.915	-3.478	1	96.3
88	CA	THR	A	19	50.377	87.008	-3.544	1	92.86
89	C	THR	A	19	50.692	86.417	-4.909	1	89.53
90	O	THR	A	19	49.833	86.358	-5.787	1	90.35
91	CB	THR	A	19	50.198	85.821	-2.584	1	93.8
92	OG1	THR	A	19	49.092	86.07	-1.707	1	96.25
93	CG2	THR	A	19	51.469	85.599	-1.762	1	94.19
94	N	ALA	A	20	51.931	85.947	-5.052	1	84.1
95	CA	ALA	A	20	52.392	85.322	-6.279	1	80.21
96	C	ALA	A	20	52.686	83.861	-6.032	1	79.19
97	O	ALA	A	20	53.447	83.499	-5.123	1	79.32
98	CB	ALA	A	20	53.616	85.993	-6.789	1	80.49
99	N	TRP	A	21	52.093	83.029	-6.877	1	77.5
100	CA	TRP	A	21	52.244	81.579	-6.794	1	77.45
101	C	TRP	A	21	53.081	81.073	-7.941	1	74.6
102	O	TRP	A	21	53.083	81.667	-9.006	1	74.48
103	CB	TRP	A	21	50.883	80.906	-6.905	1	81.76
104	CG	TRP	A	21	49.905	81.312	-5.877	1	85.09
105	CD1	TRP	A	21	49.461	82.578	-5.612	1	86.86
106	CD2	TRP	A	21	49.174	80.443	-5.022	1	86.32
107	NE1	TRP	A	21	48.481	82.545	-4.652	1	87.59
108	CE2	TRP	A	21	48.287	81.242	-4.272	1	87.85
109	CE3	TRP	A	21	49.173	79.058	-4.823	1	87.24
110	CZ2	TRP	A	21	47.409	80.703	-3.339	1	88.69
111	CZ3	TRP	A	21	48.297	78.522	-3.894	1	89.26
112	CH2	TRP	A	21	47.426	79.344	-3.163	1	88.37

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
113	N	GLU	A	22	53.772	79.962	-7.727	1	72.87
114	CA	GLU	A	22	54.589	79.366	-8.779	1	73.61
115	C	GLU	A	22	54.254	77.885	-8.781	1	70.43
116	O	GLU	A	22	55.052	77.054	-8.375	1	72.21
117	CB	GLU	A	22	56.095	79.588	-8.526	1	78.55
118	CG	GLU	A	22	57.01	79.326	-9.751	1	84.66
119	CD	GLU	A	22	58.516	79.511	-9.469	1	88.22
120	OE1	GLU	A	22	58.873	80.143	-8.446	1	89.24
121	OE2	GLU	A	22	59.344	79.015	-10.275	1	88.75
122	N	VAL	A	23	53.051	77.565	-9.225	1	66.88
123	CA	VAL	A	23	52.581	76.187	-9.26	1	65.06
124	C	VAL	A	23	53.091	75.411	-10.474	1	64.88
125	O	VAL	A	23	53.841	75.948	-11.284	1	66.97
126	CB	VAL	A	23	51.063	76.168	-9.269	1	63.14
127	CG1	VAL	A	23	50.547	76.87	-8.039	1	61.87
128	CG2	VAL	A	23	50.548	76.846	-10.516	1	58.02
129	N	ARG	A	24	52.716	74.139	-10.581	1	61.64
130	CA	ARG	A	24	53.142	73.344	-11.721	1	60.93
131	C	ARG	A	24	52.273	73.684	-12.899	1	60.82
132	O	ARG	A	24	51.128	74.079	-12.72	1	62.47
133	CB	ARG	A	24	53.045	71.859	-11.436	1	59.28
134	CG	ARG	A	24	54.046	71.385	-10.446	1	57.53
135	CD	ARG	A	24	53.987	69.896	-10.339	1	57.5
136	NE	ARG	A	24	54.976	69.412	-9.399	1	58.33
137	CZ	ARG	A	24	54.993	68.182	-8.913	1	60.97
138	NH1	ARG	A	24	54.076	67.305	-9.296	1	64.3
139	NH2	ARG	A	24	55.929	67.827	-8.048	1	61.56
140	N	ALA	A	25	52.821	73.512	-14.102	1	61.32
141	CA	ALA	A	25	52.12	73.819	-15.353	1	59.78
142	C	ALA	A	25	50.829	73.041	-15.486	1	56.96
143	O	ALA	A	25	49.84	73.542	-16.029	1	57.32
144	CB	ALA	A	25	53.021	73.533	-16.544	1	61.78
145	N	VAL	A	26	50.861	71.816	-14.974	1	53.53
146	CA	VAL	A	26	49.732	70.909	-14.995	1	49.24
147	C	VAL	A	26	48.516	71.425	-14.201	1	49.96
148	O	VAL	A	26	47.389	71.353	-14.687	1	46.32
149	CB	VAL	A	26	50.194	69.545	-14.528	1	47.82
150	CG1	VAL	A	26	49.905	69.307	-13.062	1	47.12
151	CG2	VAL	A	26	49.614	68.51	-15.411	1	54.88
152	N	TYR	A	27	48.755	71.961	-12.999	1	50.2
153	CA	TYR	A	27	47.696	72.532	-12.165	1	50.72
154	C	TYR	A	27	47.25	73.803	-12.861	1	51.88
155	O	TYR	A	27	48.005	74.765	-12.965	1	53.42
156	CB	TYR	A	27	48.217	72.83	-10.76	1	44.91
157	CG	TYR	A	27	48.564	71.567	-10.048	1	40.92
158	CD1	TYR	A	27	47.638	70.524	-9.97	1	38.22
159	CD2	TYR	A	27	49.825	71.371	-9.518	1	40.3
160	CE1	TYR	A	27	47.961	69.309	-9.39	1	35.92
161	CE2	TYR	A	27	50.167	70.152	-8.926	1	45.49
162	CZ	TYR	A	27	49.22	69.125	-8.869	1	42.37
163	OH	TYR	A	27	49.538	67.927	-8.288	1	41.12
164	N	ARG	A	28	46.017	73.797	-13.338	1	53.27
165	CA	ARG	A	28	45.503	74.918	-14.09	1	57.84
166	C	ARG	A	28	44.336	75.676	-13.474	1	57.15
167	O	ARG	A	28	43.803	75.275	-12.459	1	58.08
168	CB	ARG	A	28	45.18	74.42	-15.501	1	63.22

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
169	CG	ARG	A	28	46.386	73.708	-16.155	1	70.45
170	CD	ARG	A	28	46.207	73.457	-17.644	1	78.5
171	NE	ARG	A	28	45.79	74.672	-18.345	1	85.36
172	CZ	ARG	A	28	45.119	74.693	-19.497	1	87.56
173	NH1	ARG	A	28	44.788	73.559	-20.106	1	86.24
174	NH2	ARG	A	28	44.742	75.854	-20.02	1	88.04
175	N	ASP	A	29	43.986	76.802	-14.093	1	60.24
176	CA	ASP	A	29	42.898	77.688	-13.666	1	60.05
177	C	ASP	A	29	42.793	77.908	-12.155	1	60.52
178	O	ASP	A	29	41.836	77.484	-11.526	1	63.24
179	CB	ASP	A	29	41.554	77.224	-14.241	1	61.34
180	CG	ASP	A	29	40.421	78.231	-13.985	1	66.29
181	OD1	ASP	A	29	40.714	79.436	-13.803	1	70.52
182	OD2	ASP	A	29	39.237	77.821	-13.955	1	64.84
183	N	LEU	A	30	43.771	78.596	-11.579	1	60.46
184	CA	LEU	A	30	43.779	78.865	-10.147	1	59.31
185	C	LEU	A	30	42.689	79.847	-9.722	1	61.11
186	O	LEU	A	30	42.378	80.795	-10.438	1	62.1
187	CB	LEU	A	30	45.15	79.393	-9.712	1	55.77
188	CG	LEU	A	30	46.34	78.442	-9.76	1	54.22
189	CD1	LEU	A	30	47.586	79.188	-9.334	1	57.44
190	CD2	LEU	A	30	46.114	77.282	-8.824	1	55.22
191	N	GLN	A	31	42.115	79.598	-8.547	1	64.21
192	CA	GLN	A	31	41.069	80.434	-7.962	1	63.96
193	C	GLN	A	31	41.232	80.405	-6.449	1	65.04
194	O	GLN	A	31	41.301	79.341	-5.86	1	62.91
195	CB	GLN	A	31	39.692	79.885	-8.315	1	64.63
196	CG	GLN	A	31	39.317	79.972	-9.782	1	66.81
197	CD	GLN	A	31	38.999	81.384	-10.212	1	69.14
198	OE1	GLN	A	31	39.546	81.886	-11.198	1	67.83
199	NE2	GLN	A	31	38.11	82.04	-9.469	1	68.7
200	N	PRO	A	32	41.287	81.58	-5.804	1	67.25
201	CA	PRO	A	32	41.441	81.695	-4.348	1	67.88
202	C	PRO	A	32	40.188	81.22	-3.605	1	65.58
203	O	PRO	A	32	39.088	81.238	-4.153	1	65
204	CB	PRO	A	32	41.631	83.196	-4.154	1	68.41
205	CG	PRO	A	32	40.687	83.747	-5.184	1	69.28
206	CD	PRO	A	32	41.052	82.907	-6.4	1	68.01
207	N	VAL	A	33	40.373	80.795	-2.361	1	63.5
208	CA	VAL	A	33	39.281	80.321	-1.518	1	62.28
209	C	VAL	A	33	39.604	80.58	-0.051	1	66.64
210	O	VAL	A	33	38.638	80.628	0.755	1	69.45
211	CB	VAL	A	33	39.008	78.8	-1.689	1	59.14
212	CG1	VAL	A	33	38.129	78.554	-2.889	1	59.56
213	CG2	VAL	A	33	40.317	78.021	-1.809	1	55.83
214	OXT	VAL	A	33	40.815	80.719	0.274	1	67.62
215	N	ALA	A	40	47.147	81.043	2.447	1	59.48
216	CA	ALA	A	40	46.242	81.104	1.261	1	58.1
217	C	ALA	A	40	46.223	79.775	0.482	1	57.51
218	O	ALA	A	40	47.24	79.084	0.319	1	56.32
219	CB	ALA	A	40	46.606	82.272	0.352	1	56.64
220	N	VAL	A	41	45.024	79.427	0.03	1	54.69
221	CA	VAL	A	41	44.766	78.197	-0.682	1	50.72
222	C	VAL	A	41	44.027	78.556	-1.944	1	50.04
223	O	VAL	A	41	43.247	79.512	-1.973	1	50.25
224	CB	VAL	A	41	43.863	77.271	0.178	1	51.04

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
225	CG1	VAL	A	41	43.434	76.049	-0.596	1	50.63
226	CG2	VAL	A	41	44.587	76.859	1.448	1	48.39
227	N	CYS	A	42	44.289	77.785	-2.989	1	49.24
228	CA	CYS	A	42	43.65	77.99	-4.273	1	51.1
229	C	CYS	A	42	43.018	76.715	-4.796	1	50.56
230	O	CYS	A	42	43.478	75.605	-4.514	1	52.01
231	CB	CYS	A	42	44.664	78.482	-5.306	1	53.52
232	SG	CYS	A	42	44.777	80.249	-5.429	1	57.08
233	N	SER	A	43	41.966	76.888	-5.579	1	48.19
234	CA	SER	A	43	41.291	75.764	-6.181	1	49.79
235	C	SER	A	43	41.768	75.733	-7.623	1	51.48
236	O	SER	A	43	41.6	76.697	-8.358	1	55.24
237	CB	SER	A	43	39.762	75.917	-6.095	1	46.11
238	OG	SER	A	43	39.244	76.94	-6.923	1	43.24
239	N	ALA	A	44	42.439	74.658	-8.004	1	51.27
240	CA	ALA	A	44	42.933	74.528	-9.359	1	50.45
241	C	ALA	A	44	42.276	73.32	-10.02	1	53.54
242	O	ALA	A	44	41.342	72.744	-9.472	1	56.92
243	CB	ALA	A	44	44.423	74.352	-9.327	1	52.24
244	N	VAL	A	45	42.736	72.967	-11.216	1	52.87
245	CA	VAL	A	45	42.234	71.804	-11.928	1	49.85
246	C	VAL	A	45	43.444	71.032	-12.379	1	50.26
247	O	VAL	A	45	44.381	71.626	-12.887	1	53.24
248	CB	VAL	A	45	41.499	72.188	-13.18	1	50.42
249	CG1	VAL	A	45	41.056	70.918	-13.929	1	48.88
250	CG2	VAL	A	45	40.335	73.095	-12.847	1	47.94
251	N	ASP	A	46	43.472	69.723	-12.159	1	52.8
252	CA	ASP	A	46	44.627	68.967	-12.624	1	52.12
253	C	ASP	A	46	44.399	68.883	-14.125	1	54.38
254	O	ASP	A	46	43.435	68.27	-14.577	1	55.61
255	CB	ASP	A	46	44.695	67.575	-12.002	1	49.52
256	CG	ASP	A	46	46.008	66.869	-12.304	1	51.61
257	OD1	ASP	A	46	46.696	67.264	-13.269	1	55.2
258	OD2	ASP	A	46	46.368	65.917	-11.584	1	48.33
259	N	GLY	A	47	45.246	69.571	-14.884	1	54.36
260	CA	GLY	A	47	45.104	69.592	-16.325	1	52.61
261	C	GLY	A	47	45.091	68.208	-16.919	1	52.87
262	O	GLY	A	47	44.491	67.989	-17.967	1	55.54
263	N	ARG	A	48	45.746	67.28	-16.237	1	51.72
264	CA	ARG	A	48	45.826	65.902	-16.684	1	54.21
265	C	ARG	A	48	44.537	65.08	-16.561	1	55.33
266	O	ARG	A	48	44.334	64.136	-17.331	1	59.88
267	CB	ARG	A	48	46.922	65.172	-15.915	1	54.16
268	CG	ARG	A	48	48.313	65.67	-16.187	1	53.52
269	CD	ARG	A	48	49.274	65.108	-15.175	1	49.08
270	NE	ARG	A	48	49.024	65.689	-13.867	1	50.85
271	CZ	ARG	A	48	49.732	65.422	-12.778	1	51.07
272	NH1	ARG	A	48	50.739	64.56	-12.841	1	53.13
273	NH2	ARG	A	48	49.444	66.035	-11.637	1	50.48
274	N	THR	A	49	43.672	65.41	-15.605	1	52.12
275	CA	THR	A	49	42.468	64.615	-15.422	1	51.49
276	C	THR	A	49	41.136	65.324	-15.484	1	52.42
277	O	THR	A	49	40.143	64.715	-15.876	1	54.52
278	CB	THR	A	49	42.53	63.809	-14.123	1	53.04
279	OG1	THR	A	49	42.626	64.693	-12.999	1	52.46
280	CG2	THR	A	49	43.725	62.874	-14.135	1	51.95

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
281	N	GLY	A	50	41.1	66.585	-15.07	1	52.62
282	CA	GLY	A	50	39.862	67.352	-15.112	1	52.55
283	C	GLY	A	50	39.207	67.479	-13.756	1	52.32
284	O	GLY	A	50	38.128	68.069	-13.621	1	53.3
285	N	ALA	A	51	39.883	66.926	-12.752	1	50.64
286	CA	ALA	A	51	39.431	66.92	-11.365	1	50.52
287	C	ALA	A	51	39.877	68.166	-10.59	1	52.14
288	O	ALA	A	51	41.081	68.467	-10.566	1	53.63
289	CB	ALA	A	51	39.966	65.684	-10.681	1	45.09
290	N	LYS	A	52	38.926	68.864	-9.945	1	48.65
291	CA	LYS	A	52	39.249	70.056	-9.163	1	45.14
292	C	LYS	A	52	40.142	69.618	-8.017	1	46.17
293	O	LYS	A	52	39.985	68.532	-7.439	1	45.35
294	CB	LYS	A	52	38.006	70.786	-8.634	1	43.45
295	CG	LYS	A	52	37.131	71.423	-9.709	1	50.2
296	CD	LYS	A	52	35.83	72.047	-9.172	1	53.93
297	CE	LYS	A	52	36.067	73.417	-8.544	1	58.33
298	NZ	LYS	A	52	34.789	74.037	-8.052	1	60.69
299	N	VAL	A	53	41.088	70.486	-7.698	1	45.92
300	CA	VAL	A	53	42.068	70.228	-6.669	1	44.29
301	C	VAL	A	53	42.237	71.479	-5.803	1	44.97
302	O	VAL	A	53	41.795	72.571	-6.185	1	47.43
303	CB	VAL	A	53	43.384	69.828	-7.372	1	44.62
304	CG1	VAL	A	53	44.586	70.526	-6.774	1	49.16
305	CG2	VAL	A	53	43.54	68.34	-7.335	1	42.42
306	N	ALA	A	54	42.78	71.3	-4.603	1	42.17
307	CA	ALA	A	54	43.039	72.414	-3.703	1	40.52
308	C	ALA	A	54	44.548	72.526	-3.542	1	43.59
309	O	ALA	A	54	45.222	71.529	-3.252	1	40.54
310	CB	ALA	A	54	42.392	72.182	-2.369	1	38.36
311	N	ILE	A	55	45.076	73.727	-3.786	1	46.03
312	CA	ILE	A	55	46.511	73.991	-3.671	1	45.31
313	C	ILE	A	55	46.762	75.019	-2.596	1	46.51
314	O	ILE	A	55	46.271	76.145	-2.681	1	47.39
315	CB	ILE	A	55	47.101	74.522	-4.981	1	45.99
316	CG1	ILE	A	55	46.829	73.537	-6.122	1	40.24
317	CG2	ILE	A	55	48.607	74.712	-4.835	1	46.63
318	CD1	ILE	A	55	47.34	74.043	-7.442	1	41.71
319	N	LYS	A	56	47.539	74.618	-1.594	1	48.16
320	CA	LYS	A	56	47.882	75.462	-0.454	1	49.54
321	C	LYS	A	56	49.334	75.862	-0.501	1	52.71
322	O	LYS	A	56	50.209	75.006	-0.512	1	50.43
323	CB	LYS	A	56	47.645	74.703	0.858	1	50.38
324	CG	LYS	A	56	47.957	75.5	2.112	1	46.35
325	CD	LYS	A	56	47.618	74.715	3.332	1	46.29
326	CE	LYS	A	56	47.542	75.613	4.542	1	46.07
327	NZ	LYS	A	56	47.036	74.905	5.754	1	41.31
328	N	LYS	A	57	49.581	77.166	-0.487	1	58.23
329	CA	LYS	A	57	50.939	77.706	-0.508	1	61.77
330	C	LYS	A	57	51.336	78.06	0.92	1	62.18
331	O	LYS	A	57	50.678	78.863	1.562	1	62.18
332	CB	LYS	A	57	50.99	78.95	-1.404	1	61.46
333	CG	LYS	A	57	52.283	79.76	-1.353	1	63.67
334	CD	LYS	A	57	52.172	81.017	-2.244	1	66.85
335	CE	LYS	A	57	53.323	82.015	-2.034	1	67.4
336	NZ	LYS	A	57	54.669	81.4	-2.232	1	64.73

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
337	N	LEU	A	58	52.355	77.386	1.444	1	66.78
338	CA	LEU	A	58	52.839	77.672	2.789	1	69.76
339	C	LEU	A	58	53.453	79.067	2.742	1	73.97
340	O	LEU	A	58	54.463	79.302	2.064	1	72.46
341	CB	LEU	A	58	53.897	76.659	3.232	1	66.96
342	CG	LEU	A	58	53.463	75.428	4.023	1	67.54
343	CD1	LEU	A	58	52.732	75.852	5.276	1	67.95
344	CD2	LEU	A	58	52.596	74.518	3.184	1	66.08
345	N	TYR	A	59	52.782	79.996	3.412	1	79.16
346	CA	TYR	A	59	53.196	81.389	3.495	1	84.09
347	C	TYR	A	59	54.514	81.684	4.236	1	83.49
348	O	TYR	A	59	54.537	81.738	5.476	1	83.18
349	CB	TYR	A	59	52.095	82.18	4.22	1	89.86
350	CG	TYR	A	59	52.387	83.653	4.452	1	96.71
351	CD1	TYR	A	59	52.845	84.477	3.41	1	98.52
352	CD2	TYR	A	59	52.201	84.228	5.723	1	97.81
353	CE1	TYR	A	59	53.112	85.84	3.629	1	100
354	CE2	TYR	A	59	52.463	85.585	5.953	1	100
355	CZ	TYR	A	59	52.92	86.384	4.903	1	100
356	OH	TYR	A	59	53.201	87.715	5.13	1	99.54
357	N	ARG	A	60	55.588	81.894	3.467	1	80.81
358	CA	ARG	A	60	56.942	82.136	3.989	1	79.04
359	C	ARG	A	60	57.262	81.241	5.189	1	77.23
360	O	ARG	A	60	57.52	81.726	6.282	1	77.48
361	CB	ARG	A	60	57.146	83.614	4.354	1	78.7
362	N	PRO	A	61	57.263	79.915	4.984	1	75.75
363	CA	PRO	A	61	57.535	78.92	6.024	1	75.16
364	C	PRO	A	61	58.874	79.027	6.739	1	76.74
365	O	PRO	A	61	59.016	78.553	7.866	1	74.75
366	CB	PRO	A	61	57.406	77.602	5.267	1	75.2
367	CG	PRO	A	61	57.838	77.965	3.887	1	73.62
368	CD	PRO	A	61	57.131	79.264	3.67	1	74.21
369	N	PHE	A	62	59.854	79.652	6.095	1	79.59
370	CA	PHE	A	62	61.178	79.781	6.699	1	82.49
371	C	PHE	A	62	61.542	81.222	7.058	1	84.85
372	O	PHE	A	62	62.671	81.685	6.861	1	84.23
373	CB	PHE	A	62	62.217	79.112	5.8	1	80.91
374	CG	PHE	A	62	61.86	77.702	5.451	1	78.9
375	CD1	PHE	A	62	61.675	76.756	6.454	1	79.17
376	CD2	PHE	A	62	61.611	77.338	4.138	1	78.6
377	CE1	PHE	A	62	61.239	75.469	6.152	1	79.7
378	CE2	PHE	A	62	61.176	76.057	3.826	1	79.46
379	CZ	PHE	A	62	60.987	75.119	4.837	1	79.38
380	N	GLN	A	63	60.55	81.909	7.618	1	87.09
381	CA	GLN	A	63	60.67	83.288	8.059	1	88.09
382	C	GLN	A	63	61.031	83.287	9.551	1	89.23
383	O	GLN	A	63	61.468	84.303	10.09	1	89.69
384	CB	GLN	A	63	59.342	84.008	7.844	1	86.79
385	CG	GLN	A	63	59.392	85.501	8.076	1	90.37
386	CD	GLN	A	63	58.008	86.123	8.229	1	91.87
387	OE1	GLN	A	63	57.047	85.458	8.628	1	90.69
388	NE2	GLN	A	63	57.906	87.414	7.924	1	92.09
389	N	SER	A	64	60.851	82.142	10.209	1	88.73
390	CA	SER	A	64	61.162	82.007	11.634	1	89
391	C	SER	A	64	61.337	80.541	12.01	1	87.92
392	O	SER	A	64	61.401	79.679	11.145	1	88.84

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
393	CB	SER	A	64	60.047	82.617	12.495	1	89.8
394	OG	SER	A	64	58.882	81.807	12.478	1	90.99
395	N	GLU	A	65	61.434	80.265	13.304	1	86.8
396	CA	GLU	A	65	61.586	78.897	13.774	1	86.76
397	C	GLU	A	65	60.199	78.343	14.075	1	85.63
398	O	GLU	A	65	59.949	77.138	13.952	1	82.75
399	CB	GLU	A	65	62.447	78.859	15.039	1	88.85
400	CG	GLU	A	65	62.723	77.449	15.547	1	90.47
401	CD	GLU	A	65	63.541	77.428	16.823	1	91.83
402	OE1	GLU	A	65	64.692	77.918	16.811	1	91.06
403	OE2	GLU	A	65	63.027	76.917	17.84	1	91.98
404	N	LEU	A	66	59.312	79.24	14.504	1	85.03
405	CA	LEU	A	66	57.937	78.884	14.827	1	82.7
406	C	LEU	A	66	57.237	78.532	13.525	1	80.07
407	O	LEU	A	66	56.487	77.566	13.464	1	81.57
408	CB	LEU	A	66	57.208	80.052	15.521	1	82.72
409	CG	LEU	A	66	55.744	79.853	15.958	1	81.69
410	CD1	LEU	A	66	55.678	78.924	17.166	1	80.22
411	CD2	LEU	A	66	55.079	81.191	16.286	1	80.13
412	N	PHE	A	67	57.498	79.303	12.479	1	77.41
413	CA	PHE	A	67	56.875	79.035	11.191	1	76.85
414	C	PHE	A	67	57.401	77.74	10.571	1	75.25
415	O	PHE	A	67	56.617	76.893	10.117	1	75.35
416	CB	PHE	A	67	57.065	80.217	10.235	1	77.22
417	CG	PHE	A	67	56.089	81.341	10.456	1	78.26
418	CD1	PHE	A	67	55.474	81.52	11.691	1	79.82
419	CD2	PHE	A	67	55.79	82.229	9.425	1	80.64
420	CE1	PHE	A	67	54.577	82.568	11.899	1	80.89
421	CE2	PHE	A	67	54.892	83.285	9.622	1	81.11
422	CZ	PHE	A	67	54.287	83.452	10.861	1	81.63
423	N	ALA	A	68	58.722	77.577	10.597	1	71.6
424	CA	ALA	A	68	59.365	76.39	10.05	1	68.46
425	C	ALA	A	68	58.858	75.138	10.743	1	66.83
426	O	ALA	A	68	58.439	74.183	10.085	1	67.36
427	CB	ALA	A	68	60.863	76.493	10.201	1	68.03
428	N	LYS	A	69	58.868	75.161	12.07	1	63.84
429	CA	LYS	A	69	58.412	74.026	12.855	1	66.01
430	C	LYS	A	69	57	73.596	12.453	1	65.55
431	O	LYS	A	69	56.727	72.415	12.264	1	66.35
432	CB	LYS	A	69	58.468	74.355	14.356	1	68.13
433	CG	LYS	A	69	58.167	73.161	15.276	1	69.3
434	CD	LYS	A	69	58.343	73.504	16.752	1	71.56
435	CE	LYS	A	69	57.347	74.573	17.222	1	73.6
436	NZ	LYS	A	69	57.501	74.89	18.682	1	72.45
437	N	ARG	A	70	56.112	74.564	12.292	1	65.13
438	CA	ARG	A	70	54.743	74.266	11.919	1	65.16
439	C	ARG	A	70	54.672	73.674	10.513	1	64.97
440	O	ARG	A	70	54.035	72.641	10.303	1	63.41
441	CB	ARG	A	70	53.879	75.524	12.064	1	67.13
442	CG	ARG	A	70	53.753	75.954	13.527	1	67.32
443	CD	ARG	A	70	53.006	77.26	13.737	1	70.96
444	NE	ARG	A	70	52.859	77.501	15.174	1	78.02
445	CZ	ARG	A	70	52.083	78.433	15.73	1	79.23
446	NH1	ARG	A	70	51.36	79.248	14.972	1	78.6
447	NH2	ARG	A	70	52.034	78.548	17.057	1	78.22
448	N	ALA	A	71	55.39	74.289	9.576	1	62.89

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
449	CA	ALA	A	71	55.413	73.83	8.2	1	58.75
450	C	ALA	A	71	55.821	72.365	8.139	1	58.63
451	O	ALA	A	71	55.147	71.549	7.517	1	62.12
452	CB	ALA	A	71	56.355	74.67	7.397	1	54.6
453	N	TYR	A	72	56.917	72.029	8.803	1	59.16
454	CA	TYR	A	72	57.399	70.653	8.822	1	57.38
455	C	TYR	A	72	56.383	69.735	9.494	1	57.72
456	O	TYR	A	72	56.133	68.633	9.011	1	60.07
457	CB	TYR	A	72	58.763	70.571	9.518	1	55.15
458	CG	TYR	A	72	59.223	69.169	9.889	1	56.2
459	CD1	TYR	A	72	58.836	68.581	11.094	1	56.75
460	CD2	TYR	A	72	60.072	68.452	9.059	1	56.1
461	CE1	TYR	A	72	59.284	67.32	11.455	1	59.23
462	CE2	TYR	A	72	60.529	67.191	9.413	1	55.79
463	CZ	TYR	A	72	60.134	66.631	10.605	1	58.73
464	OH	TYR	A	72	60.591	65.38	10.953	1	62.36
465	N	ARG	A	73	55.798	70.177	10.605	1	57.84
466	CA	ARG	A	73	54.805	69.36	11.302	1	58.98
467	C	ARG	A	73	53.582	69.089	10.428	1	59.45
468	O	ARG	A	73	53.042	67.985	10.45	1	60.42
469	CB	ARG	A	73	54.343	70.02	12.595	1	59.06
470	CG	ARG	A	73	55.309	69.986	13.742	1	58.15
471	CD	ARG	A	73	54.492	70.074	14.992	1	59.34
472	NE	ARG	A	73	55.261	70.369	16.191	1	62.16
473	CZ	ARG	A	73	55.198	71.528	16.839	1	63.83
474	NH1	ARG	A	73	54.451	72.523	16.359	1	61.55
475	NH2	ARG	A	73	55.915	71.708	17.943	1	65.35
476	N	GLU	A	74	53.147	70.11	9.683	1	58.14
477	CA	GLU	A	74	51.994	70.007	8.781	1	55.64
478	C	GLU	A	74	52.268	69.037	7.636	1	54.71
479	O	GLU	A	74	51.427	68.195	7.309	1	54.12
480	CB	GLU	A	74	51.629	71.375	8.21	1	52.31
481	CG	GLU	A	74	50.352	71.364	7.403	1	52.21
482	CD	GLU	A	74	49.819	72.753	7.096	1	56.83
483	OE1	GLU	A	74	50.516	73.765	7.39	1	55
484	OE2	GLU	A	74	48.689	72.823	6.556	1	54.47
485	N	LEU	A	75	53.429	69.179	7.005	1	52.6
486	CA	LEU	A	75	53.796	68.283	5.928	1	51.01
487	C	LEU	A	75	53.833	66.843	6.457	1	54.72
488	O	LEU	A	75	53.061	65.985	6.008	1	54.29
489	CB	LEU	A	75	55.157	68.663	5.384	1	46.85
490	CG	LEU	A	75	55.634	67.823	4.199	1	46.71
491	CD1	LEU	A	75	54.583	67.788	3.113	1	44.45
492	CD2	LEU	A	75	56.929	68.405	3.671	1	45.07
493	N	ARG	A	76	54.68	66.622	7.463	1	54.57
494	CA	ARG	A	76	54.868	65.321	8.09	1	58.08
495	C	ARG	A	76	53.606	64.583	8.527	1	59.56
496	O	ARG	A	76	53.472	63.384	8.279	1	62.82
497	CB	ARG	A	76	55.816	65.449	9.278	1	62.65
498	CG	ARG	A	76	57.29	65.37	8.912	1	69.78
499	CD	ARG	A	76	57.787	63.926	8.83	1	74.86
500	NE	ARG	A	76	57.941	63.301	10.145	1	76.79
501	CZ	ARG	A	76	58.335	62.046	10.334	1	77.88
502	NH1	ARG	A	76	58.631	61.273	9.297	1	81.32
503	NH2	ARG	A	76	58.443	61.561	11.562	1	79.04
504	N	LEU	A	77	52.712	65.271	9.229	1	57.83

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
505	CA	LEU	A	77	51.478	64.648	9.689	1	53.05
506	C	LEU	A	77	50.576	64.294	8.503	1	53.62
507	O	LEU	A	77	49.931	63.242	8.489	1	53.17
508	CB	LEU	A	77	50.726	65.579	10.635	1	48.14
509	CG	LEU	A	77	51.398	65.899	11.956	1	46.47
510	CD1	LEU	A	77	50.762	67.127	12.558	1	45.51
511	CD2	LEU	A	77	51.287	64.739	12.889	1	44.58
512	N	LEU	A	78	50.52	65.18	7.515	1	54
513	CA	LEU	A	78	49.677	64.958	6.342	1	54.05
514	C	LEU	A	78	50.209	63.795	5.538	1	54.59
515	O	LEU	A	78	49.441	62.996	5.029	1	57.31
516	CB	LEU	A	78	49.572	66.226	5.484	1	51.25
517	CG	LEU	A	78	48.559	67.272	5.972	1	51.72
518	CD1	LEU	A	78	48.601	68.498	5.08	1	49.51
519	CD2	LEU	A	78	47.159	66.673	5.99	1	50.28
520	N	LYS	A	79	51.529	63.686	5.453	1	55
521	CA	LYS	A	79	52.144	62.59	4.731	1	54.39
522	C	LYS	A	79	51.903	61.267	5.457	1	57.12
523	O	LYS	A	79	51.818	60.221	4.822	1	59.25
524	CB	LYS	A	79	53.638	62.833	4.559	1	53.25
525	CG	LYS	A	79	53.982	63.834	3.47	1	57.31
526	CD	LYS	A	79	55.487	64.061	3.378	1	61.85
527	CE	LYS	A	79	56.26	62.734	3.196	1	64.8
528	NZ	LYS	A	79	57.754	62.904	3.194	1	61.46
529	N	HIS	A	80	51.745	61.317	6.777	1	57.54
530	CA	HIS	A	80	51.515	60.117	7.567	1	58.53
531	C	HIS	A	80	50.06	59.65	7.692	1	57
532	O	HIS	A	80	49.762	58.487	7.459	1	58.22
533	CB	HIS	A	80	52.13	60.287	8.963	1	63.78
534	CG	HIS	A	80	51.692	59.252	9.96	1	72.54
535	ND1	HIS	A	80	52.39	58.086	10.188	1	75.69
536	CD2	HIS	A	80	50.625	59.219	10.8	1	76.59
537	CE1	HIS	A	80	51.773	57.379	11.121	1	78.51
538	NE2	HIS	A	80	50.699	58.044	11.509	1	76.52
539	N	MET	A	81	49.164	60.544	8.088	1	55.91
540	CA	MET	A	81	47.765	60.188	8.307	1	52.11
541	C	MET	A	81	47.084	59.652	7.069	1	51.18
542	O	MET	A	81	47.472	60.005	5.959	1	52.82
543	CB	MET	A	81	46.98	61.394	8.839	1	54.12
544	CG	MET	A	81	47.498	62.012	10.144	1	52.22
545	SD	MET	A	81	46.569	63.514	10.586	1	47.79
546	CE	MET	A	81	46.89	64.523	9.116	1	44.95
547	N	ARG	A	82	46.101	58.767	7.266	1	47.75
548	CA	ARG	A	82	45.31	58.191	6.17	1	48.03
549	C	ARG	A	82	43.913	57.82	6.687	1	47.76
550	O	ARG	A	82	43.724	56.759	7.281	1	48.95
551	CB	ARG	A	82	46.003	56.968	5.561	1	46.76
552	N	HIS	A	83	42.943	58.708	6.463	1	45.54
553	CA	HIS	A	83	41.569	58.501	6.909	1	42.87
554	C	HIS	A	83	40.533	59.198	6.027	1	44.5
555	O	HIS	A	83	40.708	60.334	5.628	1	50.18
556	CB	HIS	A	83	41.407	58.992	8.347	1	44.03
557	CG	HIS	A	83	40.116	58.584	8.976	1	41.92
558	ND1	HIS	A	83	38.927	59.234	8.723	1	45.82
559	CD2	HIS	A	83	39.809	57.533	9.766	1	37.46
560	CE1	HIS	A	83	37.94	58.592	9.321	1	40.61

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
561	NE2	HIS	A	83	38.448	57.556	9.96	1	40.41
562	N	GLU	A	84	39.405	58.538	5.817	1	47.02
563	CA	GLU	A	84	38.315	59.045	4.995	1	50.31
564	C	GLU	A	84	37.833	60.441	5.429	1	48.46
565	O	GLU	A	84	37.189	61.159	4.658	1	51.03
566	CB	GLU	A	84	37.147	58.026	5.038	1	55.9
567	CG	GLU	A	84	36.066	58.171	3.928	1	70.58
568	CD	GLU	A	84	36.529	57.735	2.501	1	79.83
569	OE1	GLU	A	84	36.563	56.51	2.209	1	81.21
570	OE2	GLU	A	84	36.821	58.623	1.654	1	81.75
571	N	ASN	A	85	38.164	60.829	6.651	1	46.02
572	CA	ASN	A	85	37.729	62.1	7.192	1	46.01
573	C	ASN	A	85	38.863	63.06	7.541	1	44.93
574	O	ASN	A	85	38.697	63.956	8.353	1	39.85
575	CB	ASN	A	85	36.87	61.846	8.424	1	46.88
576	CG	ASN	A	85	35.616	61.07	8.105	1	47.63
577	OD1	ASN	A	85	35.427	59.943	8.573	1	46.51
578	ND2	ASN	A	85	34.741	61.671	7.307	1	48.35
579	N	VAL	A	86	40.029	62.837	6.958	1	44.98
580	CA	VAL	A	86	41.17	63.697	7.201	1	44.9
581	C	VAL	A	86	41.751	63.969	5.836	1	46.35
582	O	VAL	A	86	42.034	63.029	5.075	1	48.49
583	CB	VAL	A	86	42.23	63.007	8.085	1	47.54
584	CG1	VAL	A	86	43.422	63.942	8.327	1	41.99
585	CG2	VAL	A	86	41.607	62.561	9.419	1	43.09
586	N	ILE	A	87	41.912	65.251	5.516	1	44.44
587	CA	ILE	A	87	42.439	65.651	4.217	1	39.92
588	C	ILE	A	87	43.739	64.943	3.869	1	36.81
589	O	ILE	A	87	44.565	64.666	4.735	1	36.32
590	CB	ILE	A	87	42.627	67.182	4.118	1	37.31
591	CG1	ILE	A	87	42.612	67.591	2.654	1	36.65
592	CG2	ILE	A	87	43.897	67.624	4.791	1	35.5
593	CD1	ILE	A	87	41.289	67.258	1.966	1	36.11
594	N	GLY	A	88	43.925	64.676	2.588	1	35.21
595	CA	GLY	A	88	45.122	63.989	2.171	1	36.07
596	C	GLY	A	88	45.894	64.681	1.073	1	39.81
597	O	GLY	A	88	45.375	65.515	0.33	1	42.56
598	N	LEU	A	89	47.166	64.328	0.988	1	41.01
599	CA	LEU	A	89	48.043	64.879	-0.012	1	40.55
600	C	LEU	A	89	47.959	64.106	-1.315	1	41.14
601	O	LEU	A	89	47.919	62.882	-1.309	1	41.18
602	CB	LEU	A	89	49.478	64.853	0.51	1	38.81
603	CG	LEU	A	89	50.039	66.136	1.124	1	36.07
604	CD1	LEU	A	89	48.974	67.226	1.216	1	35.5
605	CD2	LEU	A	89	50.617	65.821	2.46	1	36.48
606	N	LEU	A	90	47.886	64.834	-2.422	1	42.87
607	CA	LEU	A	90	47.86	64.242	-3.749	1	44
608	C	LEU	A	90	49.222	64.527	-4.364	1	49.61
609	O	LEU	A	90	49.729	63.765	-5.192	1	51.69
610	CB	LEU	A	90	46.808	64.899	-4.628	1	40.97
611	CG	LEU	A	90	45.336	64.575	-4.414	1	43.8
612	CD1	LEU	A	90	44.508	65.359	-5.395	1	39.75
613	CD2	LEU	A	90	45.081	63.095	-4.597	1	44.12
614	N	ASP	A	91	49.82	65.633	-3.935	1	53.92
615	CA	ASP	A	91	51.116	66.07	-4.452	1	54.97
616	C	ASP	A	91	51.6	67.179	-3.528	1	57.31

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
617	O	ASP	A	91	50.82	67.773	-2.785	1	60.61
618	CB	ASP	A	91	50.912	66.604	-5.891	1	53.32
619	CG	ASP	A	91	52.201	67.054	-6.588	1	51.11
620	OD1	ASP	A	91	53.292	66.508	-6.328	1	52.23
621	OD2	ASP	A	91	52.102	67.95	-7.453	1	49.12
622	N	VAL	A	92	52.908	67.37	-3.511	1	58.83
623	CA	VAL	A	92	53.553	68.42	-2.741	1	61.14
624	C	VAL	A	92	54.767	68.768	-3.588	1	61.33
625	O	VAL	A	92	55.463	67.878	-4.097	1	60.24
626	CB	VAL	A	92	53.983	67.948	-1.33	1	63.19
627	CG1	VAL	A	92	54.781	66.698	-1.423	1	64.54
628	CG2	VAL	A	92	54.816	69.013	-0.644	1	62.43
629	N	PHE	A	93	55.005	70.057	-3.771	1	60.48
630	CA	PHE	A	93	56.116	70.469	-4.593	1	60.78
631	C	PHE	A	93	56.71	71.795	-4.206	1	62.75
632	O	PHE	A	93	56.156	72.522	-3.399	1	65.72
633	CB	PHE	A	93	55.654	70.55	-6.044	1	60.61
634	CG	PHE	A	93	54.602	71.611	-6.299	1	57.76
635	CD1	PHE	A	93	54.968	72.922	-6.602	1	54.62
636	CD2	PHE	A	93	53.252	71.291	-6.275	1	53.86
637	CE1	PHE	A	93	54.005	73.891	-6.88	1	51.44
638	CE2	PHE	A	93	52.279	72.262	-6.553	1	50.12
639	CZ	PHE	A	93	52.661	73.56	-6.855	1	49.84
640	N	THR	A	94	57.835	72.11	-4.832	1	65.79
641	CA	THR	A	94	58.532	73.372	-4.636	1	66.86
642	C	THR	A	94	59.221	73.728	-5.949	1	69.15
643	O	THR	A	94	59.919	72.898	-6.541	1	68.3
644	CB	THR	A	94	59.567	73.314	-3.498	1	68.11
645	OG1	THR	A	94	60.271	74.561	-3.442	1	66.88
646	CG2	THR	A	94	60.561	72.172	-3.703	1	69.02
647	N	PRO	A	95	58.969	74.944	-6.46	1	70.44
648	CA	PRO	A	95	59.543	75.445	-7.709	1	72.34
649	C	PRO	A	95	60.983	75.916	-7.519	1	76.59
650	O	PRO	A	95	61.492	76.743	-8.278	1	76.44
651	CB	PRO	A	95	58.613	76.595	-8.052	1	70.61
652	CG	PRO	A	95	58.295	77.156	-6.716	1	69.15
653	CD	PRO	A	95	58.022	75.923	-5.895	1	70.42
654	N	ASP	A	96	61.607	75.411	-6.46	1	81.15
655	CA	ASP	A	96	62.985	75.731	-6.124	1	85.89
656	C	ASP	A	96	63.795	74.46	-6.371	1	89.23
657	O	ASP	A	96	63.591	73.427	-5.719	1	89.09
658	CB	ASP	A	96	63.088	76.171	-4.657	1	87.26
659	CG	ASP	A	96	62.166	77.351	-4.321	1	88.52
660	OD1	ASP	A	96	61.895	78.193	-5.211	1	88.78
661	OD2	ASP	A	96	61.714	77.434	-3.157	1	87.39
662	N	GLU	A	97	64.702	74.548	-7.336	1	92.57
663	CA	GLU	A	97	65.538	73.426	-7.742	1	94.8
664	C	GLU	A	97	66.617	72.953	-6.762	1	95.78
665	O	GLU	A	97	67.025	71.791	-6.813	1	96.37
666	CB	GLU	A	97	66.151	73.735	-9.11	1	96.5
667	CG	GLU	A	97	65.097	73.913	-10.206	1	99.27
668	CD	GLU	A	97	65.631	74.572	-11.474	1	100
669	OE1	GLU	A	97	66.764	74.241	-11.898	1	100
670	OE2	GLU	A	97	64.904	75.418	-12.049	1	98.59
671	N	THR	A	98	67.065	73.833	-5.866	1	96.37
672	CA	THR	A	98	68.109	73.474	-4.897	1	97.94

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
673	C	THR	A	98	67.76	73.865	-3.464	1	98.61
674	O	THR	A	98	67.021	74.825	-3.24	1	100
675	CB	THR	A	98	69.457	74.157	-5.242	1	99.32
676	OG1	THR	A	98	69.295	75.584	-5.22	1	100
677	CG2	THR	A	98	69.954	73.722	-6.628	1	100
678	N	LEU	A	99	68.33	73.147	-2.497	1	98.76
679	CA	LEU	A	99	68.096	73.435	-1.077	1	98.58
680	C	LEU	A	99	68.555	74.843	-0.699	1	98.17
681	O	LEU	A	99	67.985	75.475	0.196	1	97.49
682	CB	LEU	A	99	68.82	72.412	-0.193	1	98.45
683	CG	LEU	A	99	68.935	72.699	1.314	1	98.85
684	CD1	LEU	A	99	67.591	73.085	1.918	1	97.72
685	CD2	LEU	A	99	69.513	71.48	2.027	1	99.45
686	N	ASP	A	100	69.589	75.32	-1.388	1	98.74
687	CA	ASP	A	100	70.148	76.645	-1.147	1	98.98
688	C	ASP	A	100	69.092	77.761	-1.248	1	98.38
689	O	ASP	A	100	68.933	78.546	-0.306	1	98.44
690	CB	ASP	A	100	71.322	76.902	-2.099	1	98.45
691	N	ASP	A	101	68.357	77.824	-2.361	1	96.77
692	CA	ASP	A	101	67.326	78.857	-2.511	1	96.16
693	C	ASP	A	101	65.875	78.393	-2.274	1	93.79
694	O	ASP	A	101	64.919	79.116	-2.59	1	93.07
695	CB	ASP	A	101	67.472	79.644	-3.834	1	97.52
696	CG	ASP	A	101	67.524	78.752	-5.066	1	98.89
697	OD1	ASP	A	101	68.63	78.305	-5.442	1	98.35
698	OD2	ASP	A	101	66.463	78.532	-5.685	1	100
699	N	PHE	A	102	65.732	77.214	-1.665	1	90.1
700	CA	PHE	A	102	64.436	76.619	-1.327	1	85.47
701	C	PHE	A	102	63.737	77.494	-0.301	1	83.16
702	O	PHE	A	102	63.994	77.37	0.891	1	84.51
703	CB	PHE	A	102	64.664	75.22	-0.744	1	85.53
704	CG	PHE	A	102	63.471	74.632	-0.028	1	85.34
705	CD1	PHE	A	102	62.226	74.559	-0.644	1	86.01
706	CD2	PHE	A	102	63.617	74.089	1.247	1	85.55
707	CE1	PHE	A	102	61.149	73.951	-0.003	1	85.1
708	CE2	PHE	A	102	62.548	73.479	1.895	1	85.8
709	CZ	PHE	A	102	61.313	73.407	1.269	1	85.19
710	N	THR	A	103	62.858	78.38	-0.756	1	79.68
711	CA	THR	A	103	62.163	79.263	0.167	1	77.22
712	C	THR	A	103	60.772	78.795	0.565	1	75.88
713	O	THR	A	103	60.351	79.009	1.702	1	75.73
714	CB	THR	A	103	62.075	80.7	-0.368	1	77.75
715	OG1	THR	A	103	61.275	80.724	-1.555	1	79.96
716	CG2	THR	A	103	63.464	81.237	-0.677	1	78.64
717	N	ASP	A	104	60.061	78.144	-0.352	1	74.5
718	CA	ASP	A	104	58.707	77.673	-0.05	1	72.91
719	C	ASP	A	104	58.263	76.397	-0.751	1	68.34
720	O	ASP	A	104	58.992	75.83	-1.559	1	67.75
721	CB	ASP	A	104	57.679	78.788	-0.302	1	77.02
722	CG	ASP	A	104	57.929	79.544	-1.6	1	80.09
723	OD1	ASP	A	104	58.292	78.915	-2.62	1	81.9
724	OD2	ASP	A	104	57.766	80.781	-1.593	1	82.01
725	N	PHE	A	105	57.064	75.94	-0.402	1	64.51
726	CA	PHE	A	105	56.501	74.744	-0.998	1	59.22
727	C	PHE	A	105	54.993	74.747	-0.952	1	57.83
728	O	PHE	A	105	54.387	75.38	-0.086	1	56.36

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
729	CB	PHE	A	105	57.048	73.483	-0.339	1	60.04
730	CG	PHE	A	105	56.637	73.298	1.092	1	59.53
731	CD1	PHE	A	105	57.204	74.071	2.101	1	58.67
732	CD2	PHE	A	105	55.726	72.302	1.435	1	60.43
733	CE1	PHE	A	105	56.876	73.853	3.43	1	58.7
734	CE2	PHE	A	105	55.387	72.073	2.76	1	61.55
735	CZ	PHE	A	105	55.966	72.853	3.765	1	62.44
736	N	TYR	A	106	54.403	74.009	-1.886	1	56.78
737	CA	TYR	A	106	52.958	73.908	-2.025	1	55.81
738	C	TYR	A	106	52.402	72.516	-1.712	1	55.14
739	O	TYR	A	106	53.028	71.5	-2.01	1	57.87
740	CB	TYR	A	106	52.552	74.303	-3.444	1	54.84
741	CG	TYR	A	106	52.95	75.707	-3.856	1	56.08
742	CD1	TYR	A	106	54.294	76.081	-3.961	1	57.27
743	CD2	TYR	A	106	51.981	76.648	-4.184	1	56.2
744	CE1	TYR	A	106	54.657	77.357	-4.385	1	57.12
745	CE2	TYR	A	106	52.326	77.921	-4.609	1	59.97
746	CZ	TYR	A	106	53.663	78.273	-4.708	1	61.4
747	OH	TYR	A	106	53.98	79.544	-5.138	1	63.17
748	N	LEU	A	107	51.218	72.487	-1.109	1	53.1
749	CA	LEU	A	107	50.549	71.244	-0.753	1	48.73
750	C	LEU	A	107	49.338	71.108	-1.653	1	47.83
751	O	LEU	A	107	48.596	72.075	-1.872	1	48.03
752	CB	LEU	A	107	50.085	71.261	0.715	1	46.75
753	CG	LEU	A	107	51.063	71.22	1.888	1	40.76
754	CD1	LEU	A	107	50.24	71.058	3.143	1	37.5
755	CD2	LEU	A	107	52.044	70.064	1.76	1	37.48
756	N	VAL	A	108	49.138	69.905	-2.178	1	46.88
757	CA	VAL	A	108	48.009	69.649	-3.057	1	45.15
758	C	VAL	A	108	47.071	68.598	-2.468	1	47.06
759	O	VAL	A	108	47.483	67.481	-2.158	1	48.67
760	CB	VAL	A	108	48.464	69.195	-4.447	1	42.12
761	CG1	VAL	A	108	47.31	69.231	-5.402	1	43.19
762	CG2	VAL	A	108	49.539	70.093	-4.963	1	44.55
763	N	MET	A	109	45.818	68.998	-2.268	1	47.49
764	CA	MET	A	109	44.795	68.114	-1.735	1	45.79
765	C	MET	A	109	43.597	68.19	-2.665	1	44.25
766	O	MET	A	109	43.472	69.123	-3.459	1	46.15
767	CB	MET	A	109	44.351	68.553	-0.339	1	48.67
768	CG	MET	A	109	45.454	68.705	0.676	1	49.92
769	SD	MET	A	109	45.744	70.455	0.986	1	58.39
770	CE	MET	A	109	44.059	70.98	1.494	1	44.53
771	N	PRO	A	110	42.726	67.174	-2.614	1	41.04
772	CA	PRO	A	110	41.539	67.148	-3.456	1	40.26
773	C	PRO	A	110	40.596	68.287	-3.077	1	43.35
774	O	PRO	A	110	40.508	68.664	-1.912	1	46.92
775	CB	PRO	A	110	40.932	65.794	-3.117	1	37.25
776	CG	PRO	A	110	41.426	65.508	-1.777	1	32.12
777	CD	PRO	A	110	42.829	65.932	-1.831	1	36.38
778	N	PHE	A	111	39.925	68.88	-4.05	1	44.9
779	CA	PHE	A	111	39.007	69.951	-3.708	1	47.51
780	C	PHE	A	111	37.834	69.313	-2.982	1	49.49
781	O	PHE	A	111	37.23	68.37	-3.474	1	52.02
782	CB	PHE	A	111	38.526	70.664	-4.956	1	45.19
783	CG	PHE	A	111	37.633	71.819	-4.682	1	46.14
784	CD1	PHE	A	111	38.153	73.028	-4.214	1	45.08

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
785	CD2	PHE	A	111	36.272	71.722	-4.946	1	47.21
786	CE1	PHE	A	111	37.326	74.138	-4.016	1	46.51
787	CE2	PHE	A	111	35.429	72.827	-4.75	1	53.09
788	CZ	PHE	A	111	35.964	74.042	-4.284	1	51.54
789	N	MET	A	112	37.524	69.824	-1.801	1	50.56
790	CA	MET	A	112	36.439	69.288	-1.015	1	48.58
791	C	MET	A	112	35.167	70.111	-0.943	1	48.3
792	O	MET	A	112	34.406	69.952	0	1	53.66
793	CB	MET	A	112	36.924	68.992	0.393	1	50.44
794	CG	MET	A	112	37.582	67.658	0.536	1	55.21
795	SD	MET	A	112	36.429	66.367	0.188	1	63.36
796	CE	MET	A	112	35.082	66.752	1.329	1	62.09
797	N	GLY	A	113	34.913	70.971	-1.917	1	46.06
798	CA	GLY	A	113	33.68	71.743	-1.886	1	49.08
799	C	GLY	A	113	33.795	73.136	-1.299	1	52.52
800	O	GLY	A	113	33.97	74.113	-2.051	1	55.04
801	N	THR	A	114	33.579	73.236	0.015	1	49.83
802	CA	THR	A	114	33.679	74.495	0.772	1	51.27
803	C	THR	A	114	33.915	74.078	2.207	1	49.63
804	O	THR	A	114	33.834	72.9	2.521	1	50.55
805	CB	THR	A	114	32.378	75.376	0.761	1	50.33
806	OG1	THR	A	114	31.265	74.617	1.241	1	53.18
807	CG2	THR	A	114	32.076	75.919	-0.621	1	55.28
808	N	ASP	A	115	34.206	75.041	3.071	1	47.27
809	CA	ASP	A	115	34.428	74.745	4.473	1	46.43
810	C	ASP	A	115	33.136	74.976	5.237	1	46.29
811	O	ASP	A	115	32.325	75.801	4.834	1	47.91
812	CB	ASP	A	115	35.549	75.612	5.034	1	51.48
813	CG	ASP	A	115	35.25	77.094	4.937	1	50.44
814	OD1	ASP	A	115	34.349	77.574	5.644	1	48.52
815	OD2	ASP	A	115	35.929	77.778	4.155	1	52.81
816	N	LEU	A	116	32.964	74.271	6.353	1	46.55
817	CA	LEU	A	116	31.754	74.37	7.166	1	47.95
818	C	LEU	A	116	31.354	75.806	7.512	1	49.33
819	O	LEU	A	116	30.171	76.121	7.607	1	46.66
820	CB	LEU	A	116	31.908	73.554	8.45	1	46.71
821	CG	LEU	A	116	30.608	73.242	9.198	1	46.23
822	CD1	LEU	A	116	29.69	72.401	8.323	1	44.27
823	CD2	LEU	A	116	30.916	72.522	10.5	1	47.75
824	N	GLY	A	117	32.353	76.661	7.704	1	51.04
825	CA	GLY	A	117	32.109	78.05	8.033	1	51.06
826	C	GLY	A	117	31.264	78.745	6.993	1	51.94
827	O	GLY	A	117	30.255	79.353	7.323	1	52.26
828	N	LYS	A	118	31.682	78.648	5.734	1	55.84
829	CA	LYS	A	118	30.971	79.265	4.622	1	57.26
830	C	LYS	A	118	29.635	78.575	4.437	1	57.6
831	O	LYS	A	118	28.616	79.219	4.214	1	60.23
832	CB	LYS	A	118	31.776	79.157	3.321	1	57.89
833	CG	LYS	A	118	33.095	79.911	3.322	1	65.65
834	CD	LYS	A	118	33.743	79.925	1.929	1	72.34
835	CE	LYS	A	118	35.239	80.336	1.959	1	76.97
836	NZ	LYS	A	118	35.517	81.689	2.559	1	78.9
837	N	LEU	A	119	29.642	77.257	4.529	1	56.2
838	CA	LEU	A	119	28.416	76.499	4.366	1	56.49
839	C	LEU	A	119	27.33	76.967	5.329	1	55.55
840	O	LEU	A	119	26.181	77.051	4.953	1	58.41

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
841	CB	LEU	A	119	28.705	75.009	4.558	1	56.15
842	CG	LEU	A	119	27.554	74.018	4.424	1	55.81
843	CD1	LEU	A	119	26.804	74.27	3.137	1	58.27
844	CD2	LEU	A	119	28.089	72.601	4.46	1	54.15
845	N	MET	A	120	27.713	77.333	6.547	1	57.14
846	CA	MET	A	120	26.763	77.776	7.569	1	59.71
847	C	MET	A	120	26.266	79.201	7.427	1	62.43
848	O	MET	A	120	25.229	79.563	7.982	1	62.45
849	CB	MET	A	120	27.372	77.63	8.962	1	59.46
850	CG	MET	A	120	27.575	76.207	9.433	1	54.09
851	SD	MET	A	120	27.971	76.282	11.148	1	53.4
852	CE	MET	A	120	29.672	75.842	11.164	1	50.57
853	N	LYS	A	121	27.064	80.016	6.753	1	66.75
854	CA	LYS	A	121	26.759	81.413	6.522	1	71.15
855	C	LYS	A	121	25.654	81.551	5.483	1	74.01
856	O	LYS	A	121	24.809	82.439	5.576	1	74.24
857	CB	LYS	A	121	28.029	82.116	6.049	1	71.3
858	CG	LYS	A	121	27.95	83.619	5.966	1	75.75
859	CD	LYS	A	121	29.326	84.168	5.646	1	79.68
860	CE	LYS	A	121	29.387	85.683	5.715	1	80.99
861	NZ	LYS	A	121	30.794	86.136	5.51	1	82.29
862	N	HIS	A	122	25.659	80.643	4.513	1	77.93
863	CA	HIS	A	122	24.681	80.634	3.43	1	82.53
864	C	HIS	A	122	23.38	79.928	3.793	1	83.37
865	O	HIS	A	122	22.296	80.405	3.453	1	84.28
866	CB	HIS	A	122	25.272	79.976	2.173	1	88.04
867	CG	HIS	A	122	26.441	80.713	1.58	1	96.17
868	ND1	HIS	A	122	26.95	81.881	2.115	1	97.93
869	CD2	HIS	A	122	27.21	80.435	0.497	1	98.4
870	CE1	HIS	A	122	27.979	82.287	1.392	1	97.07
871	NE2	HIS	A	122	28.158	81.428	0.405	1	99.19
872	N	GLU	A	123	23.482	78.81	4.51	1	83.41
873	CA	GLU	A	123	22.296	78.043	4.884	1	83.3
874	C	GLU	A	123	22.251	77.469	6.309	1	82.55
875	O	GLU	A	123	23.276	77.374	6.992	1	81.73
876	CB	GLU	A	123	22.093	76.919	3.872	1	83.31
877	CG	GLU	A	123	23.317	76.054	3.689	1	84.61
878	CD	GLU	A	123	23.157	75.037	2.576	1	87.3
879	OE1	GLU	A	123	23.424	75.39	1.405	1	84.97
880	OE2	GLU	A	123	22.779	73.881	2.879	1	88.03
881	N	LYS	A	124	21.033	77.163	6.77	1	81.94
882	CA	LYS	A	124	20.823	76.569	8.089	1	80.88
883	C	LYS	A	124	20.889	75.086	7.817	1	76.97
884	O	LYS	A	124	20.334	74.613	6.821	1	76.35
885	CB	LYS	A	124	19.458	76.931	8.679	1	84.45
886	CG	LYS	A	124	19.39	76.759	10.205	1	87.45
887	CD	LYS	A	124	20.477	77.588	10.902	1	90.82
888	CE	LYS	A	124	20.239	77.712	12.404	1	92.72
889	NZ	LYS	A	124	19.21	78.733	12.762	1	92.32
890	N	LEU	A	125	21.528	74.352	8.717	1	72.26
891	CA	LEU	A	125	21.717	72.938	8.512	1	67.61
892	C	LEU	A	125	20.543	71.977	8.622	1	67.65
893	O	LEU	A	125	19.974	71.575	7.607	1	67.88
894	CB	LEU	A	125	22.925	72.478	9.302	1	64.04
895	CG	LEU	A	125	24.214	73.08	8.725	1	60.3
896	CD1	LEU	A	125	25.386	72.691	9.583	1	57.58

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
897	CD2	LEU	A	125	24.441	72.617	7.287	1	55.29
898	N	GLY	A	126	20.172	71.588	9.825	1	67.54
899	CA	GLY	A	126	19.072	70.652	9.933	1	69.82
900	C	GLY	A	126	19.518	69.367	10.595	1	71.75
901	O	GLY	A	126	20.573	68.822	10.27	1	70.63
902	N	GLU	A	127	18.667	68.862	11.484	1	73.97
903	CA	GLU	A	127	18.936	67.661	12.265	1	75.92
904	C	GLU	A	127	19.748	66.546	11.631	1	72.94
905	O	GLU	A	127	20.819	66.213	12.125	1	72.42
906	CB	GLU	A	127	17.639	67.112	12.865	1	80.91
907	CG	GLU	A	127	17.025	68.048	13.897	1	87.05
908	CD	GLU	A	127	16.044	67.355	14.827	1	89.95
909	OE1	GLU	A	127	16.337	66.229	15.288	1	90.58
910	OE2	GLU	A	127	14.986	67.955	15.116	1	92.8
911	N	ASP	A	128	19.257	65.975	10.542	1	72.81
912	CA	ASP	A	128	19.973	64.879	9.899	1	73.38
913	C	ASP	A	128	21.368	65.292	9.448	1	72.23
914	O	ASP	A	128	22.338	64.566	9.694	1	73.38
915	CB	ASP	A	128	19.164	64.303	8.723	1	76.74
916	CG	ASP	A	128	18.08	63.295	9.165	1	77.99
917	OD1	ASP	A	128	17.682	63.292	10.357	1	75.87
918	OD2	ASP	A	128	17.624	62.504	8.298	1	77.29
919	N	ARG	A	129	21.461	66.471	8.827	1	71.28
920	CA	ARG	A	129	22.728	67.029	8.325	1	68.06
921	C	ARG	A	129	23.748	67.271	9.439	1	63.77
922	O	ARG	A	129	24.887	66.799	9.374	1	60.78
923	CB	ARG	A	129	22.475	68.353	7.584	1	72.15
924	CG	ARG	A	129	22.456	68.246	6.058	1	78.33
925	CD	ARG	A	129	22.037	69.537	5.322	1	87.4
926	NE	ARG	A	129	23.139	70.236	4.751	1	95.58
927	CZ	ARG	A	129	23.622	70.544	3.547	1	99.37
928	NH1	ARG	A	129	23.141	70.253	2.339	1	100
929	NH2	ARG	A	129	24.763	71.201	3.646	1	99.39
930	N	ILE	A	130	23.33	68.025	10.45	1	59.15
931	CA	ILE	A	130	24.18	68.344	11.583	1	55.33
932	C	ILE	A	130	24.747	67.091	12.218	1	56.26
933	O	ILE	A	130	25.909	67.081	12.606	1	58.43
934	CB	ILE	A	130	23.41	69.145	12.622	1	53.82
935	CG1	ILE	A	130	22.945	70.462	12.001	1	55.35
936	CG2	ILE	A	130	24.265	69.397	13.843	1	54.6
937	CD1	ILE	A	130	21.997	71.288	12.858	1	55.35
938	N	GLN	A	131	23.938	66.032	12.293	1	57.96
939	CA	GLN	A	131	24.362	64.752	12.877	1	57.75
940	C	GLN	A	131	25.443	64.097	12.042	1	56.11
941	O	GLN	A	131	26.488	63.708	12.556	1	57.65
942	CB	GLN	A	131	23.193	63.769	12.988	1	58.05
943	CG	GLN	A	131	23.615	62.429	13.583	1	60.25
944	CD	GLN	A	131	22.59	61.316	13.389	1	63.87
945	OE1	GLN	A	131	22.302	60.555	14.315	1	63.78
946	NE2	GLN	A	131	22.062	61.195	12.172	1	68.48
947	N	PHE	A	132	25.165	63.96	10.751	1	55.06
948	CA	PHE	A	132	26.098	63.339	9.822	1	50.74
949	C	PHE	A	132	27.425	64.062	9.837	1	49.52
950	O	PHE	A	132	28.479	63.439	9.941	1	52.09
951	CB	PHE	A	132	25.522	63.36	8.412	1	51.78
952	CG	PHE	A	132	26.273	62.501	7.44	1	52.91

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
953	CD1	PHE	A	132	26.813	61.281	7.846	1	55.98
954	CD2	PHE	A	132	26.43	62.897	6.114	1	50.3
955	CE1	PHE	A	132	27.502	60.463	6.947	1	55.67
956	CE2	PHE	A	132	27.111	62.096	5.206	1	52.66
957	CZ	PHE	A	132	27.651	60.874	5.621	1	55.48
958	N	LEU	A	133	27.371	65.389	9.789	1	44.97
959	CA	LEU	A	133	28.59	66.181	9.785	1	39.06
960	C	LEU	A	133	29.426	65.962	11.02	1	38.59
961	O	LEU	A	133	30.605	65.639	10.902	1	34
962	CB	LEU	A	133	28.282	67.668	9.587	1	36.47
963	CG	LEU	A	133	27.721	68.033	8.21	1	33.49
964	CD1	LEU	A	133	27.493	69.52	8.108	1	37.55
965	CD2	LEU	A	133	28.669	67.569	7.13	1	29.96
966	N	VAL	A	134	28.799	66.072	12.2	1	40.9
967	CA	VAL	A	134	29.497	65.891	13.482	1	39.65
968	C	VAL	A	134	30.038	64.473	13.681	1	44.86
969	O	VAL	A	134	31.095	64.291	14.284	1	47.17
970	CB	VAL	A	134	28.619	66.268	14.668	1	34.96
971	CG1	VAL	A	134	29.425	66.21	15.96	1	28.7
972	CG2	VAL	A	134	28.046	67.654	14.464	1	35.8
973	N	TYR	A	135	29.309	63.48	13.177	1	44.23
974	CA	TYR	A	135	29.735	62.102	13.264	1	47.58
975	C	TYR	A	135	31.095	62.005	12.583	1	49.53
976	O	TYR	A	135	32.04	61.432	13.13	1	50.28
977	CB	TYR	A	135	28.729	61.2	12.535	1	52.5
978	CG	TYR	A	135	29.086	59.735	12.572	1	53.91
979	CD1	TYR	A	135	29.414	59.107	13.774	1	56.68
980	CD2	TYR	A	135	29.116	58.979	11.408	1	58.07
981	CE1	TYR	A	135	29.766	57.755	13.815	1	57.41
982	CE2	TYR	A	135	29.47	57.62	11.436	1	60.91
983	CZ	TYR	A	135	29.793	57.02	12.645	1	58.95
984	OH	TYR	A	135	30.15	55.692	12.677	1	64.25
985	N	GLN	A	136	31.185	62.609	11.398	1	47.85
986	CA	GLN	A	136	32.4	62.618	10.608	1	45.5
987	C	GLN	A	136	33.541	63.388	11.264	1	46.31
988	O	GLN	A	136	34.702	62.979	11.164	1	50.07
989	CB	GLN	A	136	32.109	63.17	9.221	1	49.4
990	CG	GLN	A	136	30.982	62.473	8.514	1	47.41
991	CD	GLN	A	136	30.897	62.878	7.07	1	50.36
992	OE1	GLN	A	136	31.781	62.556	6.285	1	55.22
993	NE2	GLN	A	136	29.829	63.584	6.702	1	48.7
994	N	MET	A	137	33.236	64.504	11.919	1	43.82
995	CA	MET	A	137	34.29	65.255	12.608	1	44.92
996	C	MET	A	137	34.949	64.309	13.596	1	45.12
997	O	MET	A	137	36.173	64.21	13.673	1	46.05
998	CB	MET	A	137	33.704	66.41	13.419	1	38.65
999	CG	MET	A	137	33.589	67.694	12.681	1	43.6
1000	SD	MET	A	137	32.38	68.73	13.498	1	50.1
1001	CE	MET	A	137	31.132	68.848	12.246	1	41.53
1002	N	LEU	A	138	34.094	63.597	14.326	1	44.55
1003	CA	LEU	A	138	34.51	62.674	15.356	1	43.19
1004	C	LEU	A	138	35.265	61.402	14.919	1	44.47
1005	O	LEU	A	138	36.187	60.962	15.603	1	39.7
1006	CB	LEU	A	138	33.322	62.377	16.243	1	41.24
1007	CG	LEU	A	138	32.93	63.617	17.05	1	38.94
1008	CD1	LEU	A	138	31.635	63.383	17.805	1	38.16

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1009	CD2	LEU	A	138	34.04	63.949	18.014	1	36.58
1010	N	LYS	A	139	34.902	60.815	13.787	1	44.25
1011	CA	LYS	A	139	35.642	59.645	13.332	1	46.56
1012	C	LYS	A	139	37.025	60.141	12.938	1	44.45
1013	O	LYS	A	139	38.039	59.494	13.226	1	46.5
1014	CB	LYS	A	139	34.962	58.954	12.139	1	47.78
1015	CG	LYS	A	139	33.628	58.301	12.473	1	52.83
1016	CD	LYS	A	139	33.344	57.067	11.63	1	56.92
1017	CE	LYS	A	139	33.274	57.39	10.137	1	67.21
1018	NZ	LYS	A	139	33.193	56.167	9.254	1	69.28
1019	N	GLY	A	140	37.054	61.305	12.295	1	41.44
1020	CA	GLY	A	140	38.313	61.885	11.885	1	37.3
1021	C	GLY	A	140	39.137	62.143	13.119	1	38.11
1022	O	GLY	A	140	40.314	61.776	13.177	1	39.32
1023	N	LEU	A	141	38.488	62.682	14.149	1	38.56
1024	CA	LEU	A	141	39.176	62.964	15.401	1	42.52
1025	C	LEU	A	141	39.698	61.715	16.083	1	46.46
1026	O	LEU	A	141	40.857	61.678	16.482	1	50.8
1027	CB	LEU	A	141	38.284	63.71	16.369	1	38.9
1028	CG	LEU	A	141	38.71	65.138	16.657	1	37.62
1029	CD1	LEU	A	141	38.106	65.52	17.99	1	34.75
1030	CD2	LEU	A	141	40.219	65.27	16.691	1	32.26
1031	N	ARG	A	142	38.849	60.69	16.191	1	48.56
1032	CA	ARG	A	142	39.233	59.44	16.817	1	50.78
1033	C	ARG	A	142	40.478	58.898	16.154	1	52.86
1034	O	ARG	A	142	41.332	58.336	16.824	1	56.57
1035	CB	ARG	A	142	38.119	58.395	16.734	1	55.32
1036	CG	ARG	A	142	38.279	57.285	17.763	1	57.07
1037	CD	ARG	A	142	37.897	55.939	17.207	1	63.65
1038	NE	ARG	A	142	36.586	55.94	16.561	1	66.88
1039	CZ	ARG	A	142	36.189	55.007	15.697	1	72.69
1040	NH1	ARG	A	142	37.001	54	15.383	1	76.63
1041	NH2	ARG	A	142	34.996	55.086	15.121	1	71.99
1042	N	TYR	A	143	40.572	59.054	14.839	1	52.65
1043	CA	TYR	A	143	41.742	58.598	14.121	1	52.95
1044	C	TYR	A	143	42.951	59.447	14.516	1	54.05
1045	O	TYR	A	143	43.945	58.928	14.997	1	55.5
1046	CB	TYR	A	143	41.528	58.698	12.616	1	56.17
1047	CG	TYR	A	143	42.776	58.374	11.819	1	54.26
1048	CD1	TYR	A	143	43.197	57.057	11.66	1	52.3
1049	CD2	TYR	A	143	43.571	59.39	11.288	1	52.16
1050	CE1	TYR	A	143	44.381	56.757	11.002	1	52.59
1051	CE2	TYR	A	143	44.758	59.101	10.631	1	53.06
1052	CZ	TYR	A	143	45.161	57.781	10.493	1	52.48
1053	OH	TYR	A	143	46.351	57.485	9.862	1	52.78
1054	N	ILE	A	144	42.859	60.755	14.32	1	52.84
1055	CA	ILE	A	144	43.962	61.655	14.641	1	50.01
1056	C	ILE	A	144	44.504	61.418	16.043	1	53.24
1057	O	ILE	A	144	45.724	61.403	16.254	1	56.72
1058	CB	ILE	A	144	43.513	63.118	14.495	1	44.87
1059	CG1	ILE	A	144	43.101	63.375	13.06	1	37.49
1060	CG2	ILE	A	144	44.63	64.074	14.858	1	44.29
1061	CD1	ILE	A	144	42.184	64.534	12.93	1	38.97
1062	N	HIS	A	145	43.596	61.187	16.989	1	53.4
1063	CA	HIS	A	145	43.96	60.948	18.388	1	52.46
1064	C	HIS	A	145	44.546	59.571	18.668	1	52.21

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1065	O	HIS	A	145	45.54	59.449	19.375	1	52.67
1066	CB	HIS	A	145	42.76	61.191	19.294	1	50.19
1067	CG	HIS	A	145	42.404	62.635	19.439	1	50.08
1068	ND1	HIS	A	145	41.191	63.058	19.937	1	48.29
1069	CD2	HIS	A	145	43.116	63.757	19.178	1	48.9
1070	CE1	HIS	A	145	41.173	64.378	19.979	1	47.85
1071	NE2	HIS	A	145	42.328	64.827	19.524	1	46.55
1072	N	ALA	A	146	43.907	58.53	18.143	1	55.63
1073	CA	ALA	A	146	44.383	57.161	18.329	1	55.06
1074	C	ALA	A	146	45.801	57.099	17.777	1	54.86
1075	O	ALA	A	146	46.623	56.304	18.234	1	57.57
1076	CB	ALA	A	146	43.478	56.174	17.603	1	51.16
1077	N	ALA	A	147	46.077	57.968	16.808	1	51.91
1078	CA	ALA	A	147	47.385	58.047	16.189	1	50.99
1079	C	ALA	A	147	48.319	58.889	17.046	1	52.19
1080	O	ALA	A	147	49.448	59.167	16.646	1	55.85
1081	CB	ALA	A	147	47.269	58.628	14.801	1	45.44
1082	N	GLY	A	148	47.839	59.299	18.218	1	53.06
1083	CA	GLY	A	148	48.635	60.11	19.134	1	53.77
1084	C	GLY	A	148	48.864	61.564	18.744	1	53.6
1085	O	GLY	A	148	49.719	62.24	19.334	1	52.84
1086	N	ILE	A	149	48.109	62.038	17.748	1	53.9
1087	CA	ILE	A	149	48.204	63.419	17.247	1	51.44
1088	C	ILE	A	149	47.161	64.32	17.913	1	49.55
1089	O	ILE	A	149	46.113	63.845	18.372	1	46.83
1090	CB	ILE	A	149	47.966	63.456	15.702	1	50.09
1091	CG1	ILE	A	149	49.077	62.7	14.977	1	51.56
1092	CG2	ILE	A	149	47.895	64.887	15.185	1	50.53
1093	CD1	ILE	A	149	48.795	62.448	13.509	1	50.48
1094	N	ILE	A	150	47.48	65.61	18.005	1	48.52
1095	CA	ILE	A	150	46.561	66.602	18.565	1	46.97
1096	C	ILE	A	150	46.448	67.684	17.489	1	48.58
1097	O	ILE	A	150	47.469	68.126	16.927	1	50.54
1098	CB	ILE	A	150	47.058	67.16	19.906	1	45.4
1099	CG1	ILE	A	150	46.063	68.172	20.441	1	42
1100	CG2	ILE	A	150	48.435	67.777	19.764	1	46.23
1101	CD1	ILE	A	150	46.248	68.454	21.885	1	38.12
1102	N	HIS	A	151	45.208	68.07	17.173	1	45.3
1103	CA	HIS	A	151	44.963	69.027	16.109	1	41.66
1104	C	HIS	A	151	45.164	70.498	16.468	1	41.51
1105	O	HIS	A	151	45.734	71.256	15.686	1	38.81
1106	CB	HIS	A	151	43.569	68.8	15.51	1	41.5
1107	CG	HIS	A	151	43.283	69.667	14.322	1	38.77
1108	ND1	HIS	A	151	43.002	71.018	14.434	1	34.51
1109	CD2	HIS	A	151	43.332	69.4	12.996	1	37.51
1110	CE1	HIS	A	151	42.906	71.541	13.226	1	36.48
1111	NE2	HIS	A	151	43.1	70.583	12.335	1	34.1
1112	N	ARG	A	152	44.589	70.907	17.593	1	42.49
1113	CA	ARG	A	152	44.696	72.282	18.094	1	44.3
1114	C	ARG	A	152	44.091	73.432	17.286	1	42.7
1115	O	ARG	A	152	44.51	74.574	17.45	1	45.98
1116	CB	ARG	A	152	46.152	72.616	18.434	1	42.63
1117	CG	ARG	A	152	46.692	71.773	19.563	1	44.71
1118	CD	ARG	A	152	48.061	71.339	19.209	1	46
1119	NE	ARG	A	152	49.055	71.932	20.082	1	48
1120	CZ	ARG	A	152	50.197	72.456	19.653	1	44.87

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1121	NH1	ARG	A	152	50.47	72.482	18.368	1	39.28
1122	NH2	ARG	A	152	51.115	72.84	20.522	1	47.52
1123	N	ASP	A	153	43.145	73.152	16.401	1	37.86
1124	CA	ASP	A	153	42.537	74.229	15.657	1	33.03
1125	C	ASP	A	153	41.237	73.882	14.934	1	34.11
1126	O	ASP	A	153	40.935	74.422	13.858	1	30.96
1127	CB	ASP	A	153	43.536	74.834	14.681	1	35.33
1128	CG	ASP	A	153	43.171	76.265	14.312	1	38.12
1129	OD1	ASP	A	153	42.713	76.977	15.228	1	37.65
1130	OD2	ASP	A	153	43.304	76.666	13.136	1	33.42
1131	N	LEU	A	154	40.456	72.989	15.519	1	31.67
1132	CA	LEU	A	154	39.215	72.62	14.884	1	34.72
1133	C	LEU	A	154	38.261	73.801	14.986	1	33.66
1134	O	LEU	A	154	37.984	74.316	16.07	1	36.09
1135	CB	LEU	A	154	38.629	71.363	15.537	1	32.99
1136	CG	LEU	A	154	39.621	70.225	15.391	1	37.07
1137	CD1	LEU	A	154	39.04	68.954	15.949	1	38.07
1138	CD2	LEU	A	154	39.952	70.048	13.923	1	37.8
1139	N	LYS	A	155	37.817	74.275	13.84	1	33.76
1140	CA	LYS	A	155	36.886	75.388	13.785	1	33.65
1141	C	LYS	A	155	36.179	75.165	12.483	1	33.44
1142	O	LYS	A	155	36.662	74.419	11.638	1	38.45
1143	CB	LYS	A	155	37.633	76.721	13.812	1	34.17
1144	CG	LYS	A	155	38.57	76.962	12.662	1	36.29
1145	CD	LYS	A	155	39.46	78.147	12.994	1	40.9
1146	CE	LYS	A	155	40.19	78.649	11.761	1	44.08
1147	NZ	LYS	A	155	40.597	80.069	11.942	1	48.37
1148	N	PRO	A	156	35.031	75.798	12.285	1	34.12
1149	CA	PRO	A	156	34.295	75.603	11.035	1	36.23
1150	C	PRO	A	156	35.141	75.803	9.781	1	38.17
1151	O	PRO	A	156	35.019	75.056	8.801	1	44.37
1152	CB	PRO	A	156	33.173	76.632	11.146	1	38.31
1153	CG	PRO	A	156	32.977	76.791	12.656	1	32.77
1154	CD	PRO	A	156	34.387	76.82	13.132	1	36.22
1155	N	GLY	A	157	36.032	76.782	9.825	1	36.42
1156	CA	GLY	A	157	36.869	77.05	8.672	1	36.45
1157	C	GLY	A	157	37.888	75.984	8.31	1	37.09
1158	O	GLY	A	157	38.461	76.025	7.222	1	39.63
1159	N	ASN	A	158	38.189	75.092	9.243	1	35.94
1160	CA	ASN	A	158	39.134	74.022	8.98	1	38
1161	C	ASN	A	158	38.407	72.69	8.827	1	40.26
1162	O	ASN	A	158	38.937	71.653	9.224	1	40.86
1163	CB	ASN	A	158	40.154	73.878	10.098	1	40.07
1164	CG	ASN	A	158	41.023	75.098	10.258	1	43.16
1165	OD1	ASN	A	158	41.442	75.723	9.272	1	37.2
1166	ND2	ASN	A	158	41.318	75.441	11.515	1	34.89
1167	N	LEU	A	159	37.18	72.725	8.317	1	37.04
1168	CA	LEU	A	159	36.431	71.504	8.087	1	38.44
1169	C	LEU	A	159	35.781	71.608	6.719	1	39.1
1170	O	LEU	A	159	34.894	72.428	6.52	1	41.71
1171	CB	LEU	A	159	35.36	71.292	9.152	1	37.87
1172	CG	LEU	A	159	35.789	71.147	10.614	1	38.17
1173	CD1	LEU	A	159	34.536	71.153	11.472	1	31.96
1174	CD2	LEU	A	159	36.626	69.872	10.825	1	33.65
1175	N	ALA	A	160	36.217	70.766	5.784	1	38.19
1176	CA	ALA	A	160	35.68	70.784	4.428	1	41.44

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1177	C	ALA	A	160	34.483	69.84	4.243	1	43.35
1178	O	ALA	A	160	34.45	68.741	4.794	1	44.14
1179	CB	ALA	A	160	36.768	70.479	3.426	1	39.51
1180	N	VAL	A	161	33.514	70.279	3.445	1	42.13
1181	CA	VAL	A	161	32.301	69.534	3.22	1	43.71
1182	C	VAL	A	161	31.932	69.638	1.759	1	46.04
1183	O	VAL	A	161	31.724	70.74	1.273	1	50.8
1184	CB	VAL	A	161	31.125	70.168	4.04	1	45.02
1185	CG1	VAL	A	161	29.842	69.37	3.846	1	45.25
1186	CG2	VAL	A	161	31.473	70.275	5.51	1	40.03
1187	N	ASN	A	162	31.809	68.512	1.061	1	47.62
1188	CA	ASN	A	162	31.429	68.556	-0.349	1	49.32
1189	C	ASN	A	162	29.905	68.461	-0.598	1	51.11
1190	O	ASN	A	162	29.111	68.428	0.343	1	48.96
1191	CB	ASN	A	162	32.185	67.492	-1.14	1	50.43
1192	CG	ASN	A	162	31.84	66.079	-0.711	1	52.01
1193	OD1	ASN	A	162	30.747	65.82	-0.199	1	51.44
1194	ND2	ASN	A	162	32.779	65.15	-0.92	1	48.74
1195	N	GLU	A	163	29.512	68.433	-1.87	1	55.5
1196	CA	GLU	A	163	28.1	68.35	-2.278	1	61.45
1197	C	GLU	A	163	27.335	67.162	-1.671	1	60.68
1198	O	GLU	A	163	26.124	67.239	-1.46	1	58.41
1199	CB	GLU	A	163	27.988	68.234	-3.803	1	68.07
1200	CG	GLU	A	163	28.672	69.316	-4.629	1	73.73
1201	CD	GLU	A	163	28.449	69.101	-6.127	1	77.17
1202	OE1	GLU	A	163	28.698	67.969	-6.62	1	79.46
1203	OE2	GLU	A	163	28.014	70.059	-6.802	1	76.47
1204	N	ASP	A	164	28.037	66.05	-1.47	1	60.54
1205	CA	ASP	A	164	27.45	64.848	-0.894	1	61.87
1206	C	ASP	A	164	27.58	64.809	0.628	1	60.86
1207	O	ASP	A	164	27.508	63.751	1.243	1	61.26
1208	CB	ASP	A	164	28.088	63.607	-1.52	1	65.4
1209	CG	ASP	A	164	27.698	63.419	-2.985	1	70.38
1210	OD1	ASP	A	164	26.792	64.138	-3.475	1	75.26
1211	OD2	ASP	A	164	28.289	62.537	-3.65	1	72.93
1212	N	CYS	A	165	27.725	65.987	1.224	1	61.1
1213	CA	CYS	A	165	27.869	66.163	2.667	1	59.91
1214	C	CYS	A	165	28.969	65.351	3.355	1	56.36
1215	O	CYS	A	165	28.874	65.03	4.541	1	55.67
1216	CB	CYS	A	165	26.522	66.006	3.378	1	62.25
1217	SG	CYS	A	165	25.575	67.549	3.459	1	69.45
1218	N	GLU	A	166	30.027	65.049	2.611	1	53.49
1219	CA	GLU	A	166	31.156	64.314	3.156	1	51.71
1220	C	GLU	A	166	32.117	65.345	3.744	1	50.11
1221	O	GLU	A	166	32.265	66.456	3.22	1	49.13
1222	CB	GLU	A	166	31.81	63.479	2.065	1	56.51
1223	CG	GLU	A	166	30.799	62.576	1.368	1	61.45
1224	CD	GLU	A	166	31.419	61.668	0.323	1	65.93
1225	OE1	GLU	A	166	32.019	62.19	-0.637	1	64.13
1226	OE2	GLU	A	166	31.286	60.429	0.453	1	68.55
1227	N	LEU	A	167	32.735	64.998	4.864	1	45.15
1228	CA	LEU	A	167	33.616	65.93	5.53	1	40.51
1229	C	LEU	A	167	35.027	65.419	5.676	1	41
1230	O	LEU	A	167	35.252	64.219	5.774	1	40.97
1231	CB	LEU	A	167	33.032	66.3	6.905	1	39.98
1232	CG	LEU	A	167	33.838	67.137	7.921	1	38.58

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1233	CD1	LEU	A	167	32.926	67.97	8.808	1	27.71
1234	CD2	LEU	A	167	34.751	66.237	8.771	1	34.34
1235	N	LYS	A	168	35.973	66.355	5.642	1	40.86
1236	CA	LYS	A	168	37.392	66.079	5.814	1	42.41
1237	C	LYS	A	168	38.004	67.211	6.659	1	43.49
1238	O	LYS	A	168	37.774	68.406	6.403	1	46.01
1239	CB	LYS	A	168	38.098	65.929	4.46	1	42.92
1240	CG	LYS	A	168	37.872	64.56	3.787	1	44.62
1241	CD	LYS	A	168	38.198	64.587	2.296	1	52.06
1242	CE	LYS	A	168	38.285	63.188	1.673	1	57.6
1243	NZ	LYS	A	168	39.581	62.471	1.984	1	61.25
1244	N	ILE	A	169	38.672	66.826	7.741	1	39.75
1245	CA	ILE	A	169	39.303	67.784	8.636	1	41.55
1246	C	ILE	A	169	40.495	68.401	7.937	1	42.13
1247	O	ILE	A	169	41.334	67.691	7.391	1	43.01
1248	CB	ILE	A	169	39.748	67.105	9.942	1	42.17
1249	CG1	ILE	A	169	38.511	66.618	10.701	1	34.99
1250	CG2	ILE	A	169	40.62	68.051	10.78	1	40.6
1251	CD1	ILE	A	169	38.838	65.903	11.945	1	36.55
1252	N	LEU	A	170	40.547	69.729	7.938	1	42.65
1253	CA	LEU	A	170	41.627	70.449	7.274	1	40.48
1254	C	LEU	A	170	42.579	71.106	8.242	1	41.06
1255	O	LEU	A	170	42.46	70.963	9.453	1	44.82
1256	CB	LEU	A	170	41.044	71.549	6.392	1	36.56
1257	CG	LEU	A	170	40.081	71.17	5.282	1	33.24
1258	CD1	LEU	A	170	39.44	72.425	4.712	1	27.21
1259	CD2	LEU	A	170	40.827	70.367	4.212	1	35.84
1260	N	ASP	A	171	43.548	71.808	7.666	1	43.17
1261	CA	ASP	A	171	44.527	72.593	8.393	1	40.3
1262	C	ASP	A	171	45.268	71.961	9.536	1	42.45
1263	O	ASP	A	171	44.912	72.174	10.691	1	43.81
1264	CB	ASP	A	171	43.844	73.848	8.921	1	42.72
1265	CG	ASP	A	171	44.799	75.005	9.097	1	44.84
1266	OD1	ASP	A	171	46.025	74.775	9.215	1	47.06
1267	OD2	ASP	A	171	44.312	76.146	9.106	1	39.79
1268	N	PHE	A	172	46.327	71.218	9.246	1	46.22
1269	CA	PHE	A	172	47.108	70.653	10.337	1	43.13
1270	C	PHE	A	172	48.268	71.569	10.653	1	44.84
1271	O	PHE	A	172	49.223	71.164	11.295	1	50.63
1272	CB	PHE	A	172	47.57	69.249	10.004	1	40.11
1273	CG	PHE	A	172	46.511	68.227	10.222	1	42.51
1274	CD1	PHE	A	172	45.443	68.113	9.334	1	37.18
1275	CD2	PHE	A	172	46.538	67.42	11.351	1	43.32
1276	CE1	PHE	A	172	44.424	67.219	9.574	1	39.35
1277	CE2	PHE	A	172	45.509	66.507	11.602	1	42.4
1278	CZ	PHE	A	172	44.449	66.412	10.708	1	40.02
1279	N	GLY	A	173	48.127	72.835	10.269	1	45.22
1280	CA	GLY	A	173	49.171	73.821	10.489	1	46.84
1281	C	GLY	A	173	49.545	74.088	11.934	1	47.38
1282	O	GLY	A	173	50.623	74.616	12.205	1	49.51
1283	N	LEU	A	174	48.646	73.763	12.856	1	45.52
1284	CA	LEU	A	174	48.916	73.957	14.271	1	44.63
1285	C	LEU	A	174	48.941	72.605	14.969	1	44.93
1286	O	LEU	A	174	49.053	72.541	16.182	1	47.2
1287	CB	LEU	A	174	47.856	74.841	14.908	1	44.61
1288	CG	LEU	A	174	48.229	75.406	16.275	1	49.88

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1289	CD1	LEU	A	174	49.408	76.35	16.138	1	50.28
1290	CD2	LEU	A	174	47.046	76.133	16.893	1	54.32
1291	N	ALA	A	175	48.845	71.517	14.208	1	45.79
1292	CA	ALA	A	175	48.854	70.176	14.807	1	44.94
1293	C	ALA	A	175	50.243	69.692	15.171	1	44.54
1294	O	ALA	A	175	51.235	70.27	14.75	1	41.86
1295	CB	ALA	A	175	48.187	69.187	13.888	1	46.67
1296	N	ARG	A	176	50.296	68.641	15.985	1	49.19
1297	CA	ARG	A	176	51.561	68.042	16.44	1	51.9
1298	C	ARG	A	176	51.247	66.701	17.116	1	55.98
1299	O	ARG	A	176	50.073	66.283	17.216	1	51.59
1300	CB	ARG	A	176	52.271	68.948	17.464	1	51.52
1301	CG	ARG	A	176	51.857	68.668	18.925	1	55.87
1302	CD	ARG	A	176	52.19	69.783	19.899	1	61.12
1303	NE	ARG	A	176	53.611	69.945	20.212	1	62.43
1304	CZ	ARG	A	176	54.355	69.049	20.846	1	61.3
1305	NH1	ARG	A	176	53.838	67.888	21.224	1	64.17
1306	NH2	ARG	A	176	55.584	69.365	21.216	1	58.26
1307	N	GLN	A	177	52.308	66.044	17.587	1	60.36
1308	CA	GLN	A	177	52.184	64.772	18.293	1	63.98
1309	C	GLN	A	177	51.927	65.126	19.758	1	63.42
1310	O	GLN	A	177	52.665	65.916	20.353	1	60.44
1311	CB	GLN	A	177	53.48	63.968	18.168	1	67.7
1312	CG	GLN	A	177	53.409	62.558	18.744	1	74.25
1313	CD	GLN	A	177	54.789	61.941	18.914	1	79.21
1314	OE1	GLN	A	177	55.633	62.471	19.64	1	82.48
1315	NE2	GLN	A	177	55.028	60.825	18.239	1	79.83
1316	N	ALA	A	178	50.862	64.57	20.323	1	64.02
1317	CA	ALA	A	178	50.519	64.844	21.716	1	65.23
1318	C	ALA	A	178	51.662	64.478	22.66	1	66.35
1319	O	ALA	A	178	52.307	63.438	22.512	1	69.08
1320	CB	ALA	A	178	49.238	64.103	22.111	1	60.29
1321	N	ASP	A	179	51.94	65.372	23.596	1	67.31
1322	CA	ASP	A	179	52.993	65.158	24.576	1	68.71
1323	C	ASP	A	179	52.537	65.78	25.894	1	68.87
1324	O	ASP	A	179	51.394	66.21	26.01	1	70.97
1325	CB	ASP	A	179	54.304	65.777	24.083	1	71.26
1326	CG	ASP	A	179	55.52	65.295	24.869	1	73.83
1327	OD1	ASP	A	179	55.531	64.124	25.314	1	74.47
1328	OD2	ASP	A	179	56.471	66.089	25.034	1	73.49
1329	N	SER	A	180	53.411	65.817	26.891	1	69.23
1330	CA	SER	A	180	53.046	66.368	28.19	1	68.77
1331	C	SER	A	180	53.043	67.885	28.307	1	67.64
1332	O	SER	A	180	52.133	68.46	28.891	1	66.44
1333	CB	SER	A	180	53.922	65.76	29.281	1	70.3
1334	OG	SER	A	180	53.473	64.456	29.611	1	71.23
1335	N	GLU	A	181	54.052	68.534	27.748	1	68.69
1336	CA	GLU	A	181	54.143	69.984	27.823	1	71.37
1337	C	GLU	A	181	54.198	70.612	26.431	1	71.61
1338	O	GLU	A	181	55.273	70.689	25.82	1	74.1
1339	CB	GLU	A	181	55.388	70.373	28.61	1	75.55
1340	CG	GLU	A	181	55.149	71.368	29.736	1	83.03
1341	CD	GLU	A	181	56.454	71.85	30.376	1	87.43
1342	OE1	GLU	A	181	57.151	71.028	31.014	1	90.21
1343	OE2	GLU	A	181	56.787	73.05	30.235	1	87.65
1344	N	MET	A	182	53.042	71.05	25.929	1	68.51

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1345	CA	MET	A	182	52.94	71.662	24.599	1	64.13
1346	C	MET	A	182	52.932	73.194	24.612	1	61.59
1347	O	MET	A	182	52.872	73.807	25.675	1	64.31
1348	CB	MET	A	182	51.709	71.109	23.875	1	59.85
1349	CG	MET	A	182	51.801	69.609	23.696	1	56.94
1350	SD	MET	A	182	50.316	68.824	23.14	1	53.18
1351	CE	MET	A	182	49.474	68.578	24.651	1	54.19
1352	N	TPO	A	183	53.021	73.803	23.431	1	59.32
1353	CA	TPO	A	183	53.028	75.263	23.3	1	58
1354	CB	TPO	A	183	53.464	75.683	21.864	1	57.99
1355	CG2	TPO	A	183	52.956	77.088	21.485	1	58.26
1356	OG1	TPO	A	183	52.97	74.713	20.996	1	56.3
1357	P	TPO	A	183	53.924	73.74	20.272	1	55.49
1358	O1P	TPO	A	183	53.848	72.446	20.99	1	45.8
1359	O2P	TPO	A	183	55.271	74.333	20.324	1	54.53
1360	O3P	TPO	A	183	53.385	73.561	18.894	1	49.97
1361	C	TPO	A	183	51.691	75.873	23.781	1	57
1362	O	TPO	A	183	50.611	75.331	23.535	1	56.36
1363	N	GLY	A	184	51.804	76.966	24.533	1	55.74
1364	CA	GLY	A	184	50.66	77.612	25.145	1	51.9
1365	C	GLY	A	184	49.537	78.229	24.343	1	53.51
1366	O	GLY	A	184	48.381	77.829	24.499	1	54.51
1367	N	PTR	A	185	49.836	79.254	23.553	1	49.84
1368	CA	PTR	A	185	48.793	79.908	22.779	1	49.06
1369	C	PTR	A	185	48.389	79.089	21.547	1	48.67
1370	O	PTR	A	185	48.974	79.231	20.469	1	48.26
1371	CB	PTR	A	185	49.251	81.311	22.385	1	51.6
1372	CG	PTR	A	185	48.096	82.259	22.464	1	50.44
1373	CD1	PTR	A	185	47.895	83.132	21.354	1	53.05
1374	CD2	PTR	A	185	47.219	82.274	23.574	1	49.54
1375	CE1	PTR	A	185	46.807	84.037	21.331	1	50.75
1376	CE2	PTR	A	185	46.129	83.18	23.553	1	49.06
1377	CZ	PTR	A	185	45.936	84.047	22.439	1	52.04
1378	OH	PTR	A	185	44.93	84.97	22.508	1	54.28
1379	P	PTR	A	185	43.857	85.166	21.396	1	57.49
1380	O1P	PTR	A	185	44.167	84.404	20.185	1	59.75
1381	O2P	PTR	A	185	43.939	86.616	21.029	1	55.95
1382	O3P	PTR	A	185	42.56	84.882	21.969	1	52.04
1383	N	VAL	A	186	47.394	78.224	21.719	1	43.44
1384	CA	VAL	A	186	46.934	77.368	20.63	1	43.98
1385	C	VAL	A	186	45.399	77.374	20.506	1	43.27
1386	O	VAL	A	186	44.709	77.71	21.459	1	43.93
1387	CB	VAL	A	186	47.453	75.918	20.82	1	45.53
1388	CG1	VAL	A	186	48.985	75.906	20.878	1	41.3
1389	CG2	VAL	A	186	46.861	75.297	22.085	1	41.14
1390	N	VAL	A	187	44.876	76.987	19.339	1	42.53
1391	CA	VAL	A	187	43.424	76.965	19.044	1	39.94
1392	C	VAL	A	187	42.882	78.366	18.846	1	40.34
1393	O	VAL	A	187	43.285	79.282	19.544	1	42.95
1394	CB	VAL	A	187	42.552	76.336	20.154	1	35.61
1395	CG1	VAL	A	187	41.151	76.138	19.63	1	28.79
1396	CG2	VAL	A	187	43.126	75.015	20.638	1	40.37
1397	N	THR	A	188	41.973	78.537	17.894	1	41.92
1398	CA	THR	A	188	41.383	79.843	17.653	1	40.96
1399	C	THR	A	188	40.489	80.137	18.835	1	42.63
1400	O	THR	A	188	39.72	79.274	19.256	1	42.64

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1401	CB	THR	A	188	40.589	79.88	16.351	1	43.57
1402	OG1	THR	A	188	41.488	79.684	15.247	1	44.23
1403	CG2	THR	A	188	39.871	81.233	16.185	1	39.7
1404	N	ARG	A	189	40.589	81.364	19.356	1	47.22
1405	CA	ARG	A	189	39.832	81.805	20.541	1	46.27
1406	C	ARG	A	189	38.411	81.281	20.796	1	43.48
1407	O	ARG	A	189	38.168	80.638	21.809	1	43.66
1408	CB	ARG	A	189	39.832	83.337	20.661	1	44.74
1409	CG	ARG	A	189	39.276	83.826	22.001	1	44.51
1410	CD	ARG	A	189	39.046	85.319	22.042	1	50.52
1411	NE	ARG	A	189	40.285	86.078	21.856	1	52.32
1412	CZ	ARG	A	189	40.414	87.123	21.041	1	48.94
1413	NH1	ARG	A	189	39.377	87.551	20.338	1	46.67
1414	NH2	ARG	A	189	41.593	87.711	20.897	1	49
1415	N	TRP	A	190	37.472	81.54	19.899	1	42.94
1416	CA	TRP	A	190	36.1	81.095	20.16	1	47.7
1417	C	TRP	A	190	35.934	79.58	20.28	1	46.92
1418	O	TRP	A	190	34.914	79.111	20.771	1	45.1
1419	CB	TRP	A	190	35.109	81.689	19.133	1	51.97
1420	CG	TRP	A	190	35.14	83.211	19.07	1	60.34
1421	CD1	TRP	A	190	35.588	84.059	20.042	1	61.7
1422	CD2	TRP	A	190	34.766	84.045	17.962	1	65.03
1423	NE1	TRP	A	190	35.526	85.36	19.613	1	64.05
1424	CE2	TRP	A	190	35.024	85.384	18.341	1	67.03
1425	CE3	TRP	A	190	34.243	83.791	16.684	1	69.62
1426	CZ2	TRP	A	190	34.777	86.469	17.49	1	68.94
1427	CZ3	TRP	A	190	33.998	84.875	15.832	1	71.43
1428	CH2	TRP	A	190	34.267	86.199	16.244	1	71.73
1429	N	TYR	A	191	36.958	78.818	19.9	1	45.76
1430	CA	TYR	A	191	36.87	77.358	19.95	1	44.82
1431	C	TYR	A	191	37.866	76.795	20.928	1	45.92
1432	O	TYR	A	191	37.965	75.582	21.129	1	47.32
1433	CB	TYR	A	191	37.074	76.77	18.551	1	45.18
1434	CG	TYR	A	191	36.101	77.347	17.549	1	44.44
1435	CD1	TYR	A	191	34.805	76.844	17.441	1	45.23
1436	CD2	TYR	A	191	36.431	78.484	16.807	1	46.36
1437	CE1	TYR	A	191	33.857	77.471	16.632	1	46.26
1438	CE2	TYR	A	191	35.491	79.113	15.999	1	44.56
1439	CZ	TYR	A	191	34.213	78.606	15.925	1	44.09
1440	OH	TYR	A	191	33.284	79.254	15.17	1	50.17
1441	N	ARG	A	192	38.553	77.709	21.597	1	47.41
1442	CA	ARG	A	192	39.555	77.373	22.588	1	45.02
1443	C	ARG	A	192	38.92	76.95	23.916	1	47.93
1444	O	ARG	A	192	38.024	77.608	24.442	1	51.1
1445	CB	ARG	A	192	40.475	78.57	22.786	1	41.99
1446	CG	ARG	A	192	41.584	78.332	23.742	1	40.62
1447	CD	ARG	A	192	42.805	79.03	23.235	1	43.71
1448	NE	ARG	A	192	42.746	80.46	23.469	1	48.59
1449	CZ	ARG	A	192	43.082	81.378	22.579	1	49.04
1450	NH1	ARG	A	192	43.491	81.023	21.374	1	45.98
1451	NH2	ARG	A	192	43.089	82.654	22.93	1	56.7
1452	N	ALA	A	193	39.371	75.818	24.436	1	48.22
1453	CA	ALA	A	193	38.869	75.295	25.688	1	44.88
1454	C	ALA	A	193	39.508	76.082	26.807	1	44.69
1455	O	ALA	A	193	40.666	76.484	26.71	1	48.77
1456	CB	ALA	A	193	39.229	73.835	25.817	1	42.35

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1457	N	PRO	A	194	38.792	76.243	27.924	1	43.42
1458	CA	PRO	A	194	39.31	76.989	29.071	1	42.8
1459	C	PRO	A	194	40.691	76.564	29.592	1	44.92
1460	O	PRO	A	194	41.541	77.421	29.911	1	45.24
1461	CB	PRO	A	194	38.217	76.794	30.12	1	39.72
1462	CG	PRO	A	194	37.561	75.517	29.702	1	42.17
1463	CD	PRO	A	194	37.483	75.65	28.237	1	38.63
1464	N	GLU	A	195	40.943	75.259	29.64	1	43.82
1465	CA	GLU	A	195	42.215	74.81	30.171	1	40.22
1466	C	GLU	A	195	43.414	75.237	29.371	1	38.03
1467	O	GLU	A	195	44.526	75.174	29.874	1	34.35
1468	CB	GLU	A	195	42.231	73.305	30.443	1	42.63
1469	CG	GLU	A	195	42.296	72.44	29.238	1	44.64
1470	CD	GLU	A	195	40.954	72.224	28.571	1	49.9
1471	OE1	GLU	A	195	39.9	72.67	29.096	1	50.67
1472	OE2	GLU	A	195	40.968	71.587	27.498	1	50.63
1473	N	VAL	A	196	43.21	75.708	28.142	1	40.58
1474	CA	VAL	A	196	44.36	76.166	27.357	1	44.46
1475	C	VAL	A	196	44.997	77.345	28.104	1	48.11
1476	O	VAL	A	196	46.2	77.606	27.997	1	50.59
1477	CB	VAL	A	196	43.965	76.621	25.944	1	42.44
1478	CG1	VAL	A	196	45.201	77.098	25.184	1	40.12
1479	CG2	VAL	A	196	43.298	75.48	25.198	1	41.61
1480	N	ILE	A	197	44.176	78.018	28.908	1	48.55
1481	CA	ILE	A	197	44.633	79.15	29.68	1	46.36
1482	C	ILE	A	197	44.757	78.862	31.169	1	45
1483	O	ILE	A	197	45.778	79.186	31.778	1	44.15
1484	CB	ILE	A	197	43.753	80.354	29.402	1	47.63
1485	CG1	ILE	A	197	43.949	80.746	27.941	1	44.16
1486	CG2	ILE	A	197	44.118	81.523	30.327	1	49.36
1487	CD1	ILE	A	197	43.114	81.88	27.533	1	52.88
1488	N	LEU	A	198	43.742	78.241	31.757	1	43.62
1489	CA	LEU	A	198	43.807	77.903	33.176	1	46.21
1490	C	LEU	A	198	44.936	76.915	33.436	1	49.78
1491	O	LEU	A	198	45.58	76.949	34.482	1	53.09
1492	CB	LEU	A	198	42.491	77.304	33.665	1	43.96
1493	CG	LEU	A	198	41.284	78.234	33.487	1	48.66
1494	CD1	LEU	A	198	40.06	77.679	34.234	1	37.35
1495	CD2	LEU	A	198	41.664	79.652	33.977	1	43.46
1496	N	ASN	A	199	45.178	76.044	32.462	1	52.51
1497	CA	ASN	A	199	46.217	75.042	32.566	1	52.27
1498	C	ASN	A	199	47.276	75.249	31.508	1	52.19
1499	O	ASN	A	199	47.615	74.329	30.782	1	55.24
1500	CB	ASN	A	199	45.614	73.642	32.428	1	54.1
1501	CG	ASN	A	199	46.574	72.559	32.856	1	55
1502	OD1	ASN	A	199	47.741	72.839	33.178	1	47.2
1503	ND2	ASN	A	199	46.092	71.315	32.879	1	55.42
1504	N	TRP	A	200	47.823	76.454	31.459	1	53.79
1505	CA	TRP	A	200	48.861	76.824	30.496	1	55.23
1506	C	TRP	A	200	49.845	75.687	30.219	1	56.22
1507	O	TRP	A	200	50.379	75.081	31.153	1	57.24
1508	CB	TRP	A	200	49.623	78.037	31.019	1	51.9
1509	CG	TRP	A	200	50.569	78.629	30.051	1	52.56
1510	CD1	TRP	A	200	51.938	78.625	30.125	1	53.16
1511	CD2	TRP	A	200	50.228	79.384	28.885	1	51.63
1512	NE1	TRP	A	200	52.472	79.347	29.07	1	52.41

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1513	CE2	TRP	A	200	51.444	79.822	28.298	1	51.06
1514	CE3	TRP	A	200	49.018	79.74	28.28	1	48.62
1515	CZ2	TRP	A	200	51.474	80.597	27.138	1	50.38
1516	CZ3	TRP	A	200	49.051	80.512	27.127	1	48.8
1517	CH2	TRP	A	200	50.274	80.934	26.567	1	47.32
1518	N	MET	A	201	49.994	75.362	28.932	1	56.44
1519	CA	MET	A	201	50.899	74.322	28.421	1	53.74
1520	C	MET	A	201	50.652	72.856	28.789	1	53.26
1521	O	MET	A	201	51.457	71.998	28.416	1	53.36
1522	CB	MET	A	201	52.353	74.674	28.741	1	51.39
1523	CG	MET	A	201	52.822	75.945	28.1	1	52.93
1524	SD	MET	A	201	54.585	76.266	28.35	1	57.67
1525	CE	MET	A	201	54.759	77.836	27.394	1	54.12
1526	N	ARG	A	202	49.549	72.545	29.468	1	48.76
1527	CA	ARG	A	202	49.305	71.159	29.848	1	49.12
1528	C	ARG	A	202	47.927	70.604	29.522	1	50.94
1529	O	ARG	A	202	47.401	69.76	30.252	1	52.21
1530	CB	ARG	A	202	49.613	70.952	31.33	1	51.67
1531	CG	ARG	A	202	51.028	71.375	31.726	1	53.45
1532	CD	ARG	A	202	51.303	71.081	33.186	1	54.45
1533	NE	ARG	A	202	52.706	71.309	33.524	1	59.92
1534	CZ	ARG	A	202	53.184	72.441	34.034	1	60.71
1535	NH1	ARG	A	202	52.361	73.459	34.275	1	63.06
1536	NH2	ARG	A	202	54.485	72.559	34.288	1	55.04
1537	N	TYR	A	203	47.34	71.091	28.433	1	51.16
1538	CA	TYR	A	203	46.035	70.622	27.967	1	50.51
1539	C	TYR	A	203	46.277	69.312	27.212	1	51.12
1540	O	TYR	A	203	47.418	68.937	26.951	1	49.65
1541	CB	TYR	A	203	45.43	71.641	27.01	1	44.92
1542	CG	TYR	A	203	46.398	72.03	25.929	1	41.85
1543	CD1	TYR	A	203	47.29	73.073	26.126	1	44.76
1544	CD2	TYR	A	203	46.445	71.348	24.717	1	42.63
1545	CE1	TYR	A	203	48.216	73.435	25.144	1	46.08
1546	CE2	TYR	A	203	47.365	71.704	23.732	1	43.91
1547	CZ	TYR	A	203	48.245	72.755	23.962	1	43.02
1548	OH	TYR	A	203	49.143	73.143	23.013	1	48.44
1549	N	THR	A	204	45.206	68.631	26.837	1	51.91
1550	CA	THR	A	204	45.353	67.381	26.112	1	53.02
1551	C	THR	A	204	44.521	67.339	24.848	1	53.44
1552	O	THR	A	204	43.982	68.348	24.403	1	54.4
1553	CB	THR	A	204	44.992	66.157	26.978	1	52.28
1554	OG1	THR	A	204	43.626	66.228	27.379	1	50.51
1555	CG2	THR	A	204	45.861	66.085	28.194	1	53.26
1556	N	GLN	A	205	44.423	66.147	24.272	1	51.77
1557	CA	GLN	A	205	43.671	65.952	23.059	1	47.48
1558	C	GLN	A	205	42.221	66.284	23.296	1	47.68
1559	O	GLN	A	205	41.445	66.363	22.356	1	51.93
1560	CB	GLN	A	205	43.783	64.514	22.612	1	48.68
1561	CG	GLN	A	205	45.191	63.988	22.561	1	55.89
1562	CD	GLN	A	205	45.222	62.55	22.116	1	53.57
1563	OE1	GLN	A	205	44.566	61.692	22.704	1	58.78
1564	NE2	GLN	A	205	45.947	62.285	21.054	1	50.87
1565	N	THR	A	206	41.823	66.431	24.552	1	48.65
1566	CA	THR	A	206	40.428	66.768	24.813	1	46.66
1567	C	THR	A	206	40.084	68.191	24.363	1	43.42
1568	O	THR	A	206	38.904	68.518	24.225	1	44.4

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1569	CB	THR	A	206	40.041	66.601	26.288	1	47.5
1570	OG1	THR	A	206	41.097	67.087	27.128	1	46.28
1571	CG2	THR	A	206	39.718	65.163	26.588	1	46.28
1572	N	VAL	A	207	41.099	69.026	24.133	1	35.84
1573	CA	VAL	A	207	40.833	70.378	23.695	1	35.15
1574	C	VAL	A	207	40.127	70.341	22.361	1	38.57
1575	O	VAL	A	207	39.278	71.196	22.089	1	40.83
1576	CB	VAL	A	207	42.085	71.257	23.578	1	32.83
1577	CG1	VAL	A	207	42.909	71.118	24.788	1	36.23
1578	CG2	VAL	A	207	42.86	70.97	22.327	1	25.7
1579	N	ASP	A	208	40.44	69.325	21.553	1	39.59
1580	CA	ASP	A	208	39.82	69.159	20.237	1	38.84
1581	C	ASP	A	208	38.353	68.767	20.424	1	38.51
1582	O	ASP	A	208	37.529	68.978	19.546	1	42.24
1583	CB	ASP	A	208	40.553	68.078	19.413	1	41.46
1584	CG	ASP	A	208	41.987	68.475	19.019	1	47.15
1585	OD1	ASP	A	208	42.281	69.691	18.87	1	52.58
1586	OD2	ASP	A	208	42.825	67.568	18.821	1	46.19
1587	N	ILE	A	209	38.027	68.159	21.558	1	39.36
1588	CA	ILE	A	209	36.639	67.793	21.816	1	43.32
1589	C	ILE	A	209	35.886	69.057	22.188	1	43.82
1590	O	ILE	A	209	34.718	69.21	21.846	1	46.67
1591	CB	ILE	A	209	36.502	66.733	22.934	1	44.35
1592	CG1	ILE	A	209	37.085	65.408	22.455	1	44.48
1593	CG2	ILE	A	209	35.041	66.512	23.292	1	44.55
1594	CD1	ILE	A	209	36.376	64.872	21.245	1	48.72
1595	N	TRP	A	210	36.567	69.974	22.867	1	44.58
1596	CA	TRP	A	210	35.952	71.235	23.238	1	44.7
1597	C	TRP	A	210	35.56	71.921	21.938	1	46.84
1598	O	TRP	A	210	34.385	72.195	21.707	1	48.19
1599	CB	TRP	A	210	36.92	72.114	24.034	1	46.84
1600	CG	TRP	A	210	36.274	73.413	24.467	1	47.76
1601	CD1	TRP	A	210	36.216	74.577	23.75	1	50.28
1602	CD2	TRP	A	210	35.514	73.641	25.658	1	45.56
1603	NE1	TRP	A	210	35.451	75.504	24.413	1	50.26
1604	CE2	TRP	A	210	35.007	74.956	25.587	1	48.25
1605	CE3	TRP	A	210	35.204	72.859	26.776	1	45.53
1606	CZ2	TRP	A	210	34.209	75.507	26.59	1	46.57
1607	CZ3	TRP	A	210	34.41	73.405	27.775	1	45.12
1608	CH2	TRP	A	210	33.921	74.718	27.672	1	48.42
1609	N	SER	A	211	36.544	72.137	21.065	1	46.81
1610	CA	SER	A	211	36.308	72.765	19.769	1	43.53
1611	C	SER	A	211	35.138	72.107	19.041	1	44
1612	O	SER	A	211	34.242	72.796	18.551	1	46.51
1613	CB	SER	A	211	37.571	72.707	18.92	1	43.53
1614	OG	SER	A	211	38.633	73.428	19.535	1	40.65
1615	N	VAL	A	212	35.105	70.778	19.002	1	39.83
1616	CA	VAL	A	212	33.981	70.097	18.344	1	34.15
1617	C	VAL	A	212	32.631	70.45	18.997	1	31.62
1618	O	VAL	A	212	31.613	70.506	18.338	1	29.16
1619	CB	VAL	A	212	34.19	68.574	18.336	1	28.26
1620	CG1	VAL	A	212	32.964	67.879	17.829	1	26.78
1621	CG2	VAL	A	212	35.343	68.245	17.417	1	31.42
1622	N	GLY	A	213	32.629	70.683	20.301	1	33.4
1623	CA	GLY	A	213	31.392	71.036	20.973	1	35.22
1624	C	GLY	A	213	30.918	72.426	20.56	1	37.95

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1625	O	GLY	A	213	29.744	72.615	20.289	1	35.24
1626	N	CYS	A	214	31.834	73.392	20.538	1	37.44
1627	CA	CYS	A	214	31.508	74.749	20.147	1	41.88
1628	C	CYS	A	214	31.043	74.72	18.702	1	40.71
1629	O	CYS	A	214	30.112	75.433	18.307	1	39.35
1630	CB	CYS	A	214	32.745	75.643	20.252	1	41.96
1631	SG	CYS	A	214	33.384	75.795	21.892	1	39.81
1632	N	ILE	A	215	31.7	73.886	17.913	1	37.31
1633	CA	ILE	A	215	31.339	73.782	16.507	1	38.73
1634	C	ILE	A	215	29.956	73.153	16.373	1	38.02
1635	O	ILE	A	215	29.1	73.682	15.688	1	42.97
1636	CB	ILE	A	215	32.409	72.992	15.684	1	32.03
1637	CG1	ILE	A	215	33.782	73.656	15.818	1	33.57
1638	CG2	ILE	A	215	32.071	73.014	14.236	1	31.47
1639	CD1	ILE	A	215	34.962	72.869	15.198	1	24.34
1640	N	MET	A	216	29.722	72.035	17.044	1	42.7
1641	CA	MET	A	216	28.414	71.385	16.965	1	45.15
1642	C	MET	A	216	27.326	72.326	17.486	1	44.3
1643	O	MET	A	216	26.244	72.404	16.935	1	45
1644	CB	MET	A	216	28.397	70.087	17.769	1	42.87
1645	CG	MET	A	216	27.181	69.246	17.493	1	46.65
1646	SD	MET	A	216	26.807	68.048	18.765	1	48.35
1647	CE	MET	A	216	25.21	67.551	18.193	1	52.21
1648	N	ALA	A	217	27.641	73.06	18.539	1	46.2
1649	CA	ALA	A	217	26.706	73.989	19.14	1	44.76
1650	C	ALA	A	217	26.377	75.105	18.157	1	48.08
1651	O	ALA	A	217	25.232	75.528	18.056	1	49.39
1652	CB	ALA	A	217	27.311	74.562	20.395	1	46.54
1653	N	GLU	A	218	27.387	75.553	17.41	1	49.97
1654	CA	GLU	A	218	27.221	76.619	16.433	1	47.93
1655	C	GLU	A	218	26.371	76.173	15.268	1	49.11
1656	O	GLU	A	218	25.577	76.952	14.743	1	52
1657	CB	GLU	A	218	28.574	77.097	15.924	1	46.1
1658	CG	GLU	A	218	28.487	78.409	15.194	1	47.97
1659	CD	GLU	A	218	29.831	78.956	14.768	1	47.47
1660	OE1	GLU	A	218	30.825	78.726	15.481	1	44.18
1661	OE2	GLU	A	218	29.882	79.637	13.721	1	48.14
1662	N	MET	A	219	26.554	74.935	14.833	1	48.28
1663	CA	MET	A	219	25.76	74.427	13.727	1	50.18
1664	C	MET	A	219	24.273	74.473	14.092	1	55.31
1665	O	MET	A	219	23.442	74.875	13.278	1	60.29
1666	CB	MET	A	219	26.156	72.996	13.397	1	46.12
1667	CG	MET	A	219	27.522	72.854	12.822	1	40.5
1668	SD	MET	A	219	28.039	71.143	12.889	1	39.2
1669	CE	MET	A	219	27.603	70.545	11.311	1	39.33
1670	N	ILE	A	220	23.95	74.109	15.333	1	57.04
1671	CA	ILE	A	220	22.564	74.082	15.806	1	57.34
1672	C	ILE	A	220	21.914	75.458	16.006	1	58.12
1673	O	ILE	A	220	20.817	75.71	15.512	1	56.89
1674	CB	ILE	A	220	22.454	73.302	17.128	1	55.22
1675	CG1	ILE	A	220	23.106	71.93	16.982	1	52.68
1676	CG2	ILE	A	220	21	73.13	17.501	1	57.26
1677	CD1	ILE	A	220	23.204	71.173	18.267	1	52.7
1678	N	THR	A	221	22.575	76.317	16.778	1	58.79
1679	CA	THR	A	221	22.064	77.651	17.067	1	57.98
1680	C	THR	A	221	22.22	78.605	15.904	1	58.94

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1681	O	THR	A	221	21.296	79.333	15.573	1	64.25
1682	CB	THR	A	221	22.782	78.293	18.256	1	57.73
1683	OG1	THR	A	221	24.127	78.607	17.885	1	56.32
1684	CG2	THR	A	221	22.777	77.357	19.464	1	58.26
1685	N	GLY	A	222	23.407	78.618	15.31	1	59.14
1686	CA	GLY	A	222	23.687	79.505	14.198	1	56.36
1687	C	GLY	A	222	24.582	80.643	14.652	1	55.05
1688	O	GLY	A	222	25.162	81.36	13.845	1	55.58
1689	N	LYS	A	223	24.713	80.785	15.962	1	54.94
1690	CA	LYS	A	223	25.526	81.831	16.556	1	56.18
1691	C	LYS	A	223	26.764	81.202	17.174	1	57.53
1692	O	LYS	A	223	26.759	80.029	17.531	1	59.83
1693	CB	LYS	A	223	24.709	82.569	17.648	1	54.06
1694	N	THR	A	224	27.833	81.979	17.277	1	58.39
1695	CA	THR	A	224	29.065	81.505	17.894	1	57.22
1696	C	THR	A	224	28.724	81.331	19.373	1	59.77
1697	O	THR	A	224	28.139	82.233	19.984	1	62.77
1698	CB	THR	A	224	30.161	82.544	17.736	1	55.38
1699	OG1	THR	A	224	30.399	82.741	16.341	1	55.02
1700	CG2	THR	A	224	31.436	82.108	18.435	1	51.61
1701	N	LEU	A	225	29.09	80.181	19.943	1	59.25
1702	CA	LEU	A	225	28.768	79.863	21.332	1	55.72
1703	C	LEU	A	225	29.428	80.748	22.359	1	52.47
1704	O	LEU	A	225	28.741	81.315	23.198	1	53.73
1705	CB	LEU	A	225	29.03	78.38	21.638	1	54.46
1706	CG	LEU	A	225	28.621	77.909	23.038	1	55.79
1707	CD1	LEU	A	225	27.169	78.259	23.299	1	55.88
1708	CD2	LEU	A	225	28.844	76.42	23.185	1	52.89
1709	N	PHE	A	226	30.747	80.861	22.31	1	49.89
1710	CA	PHE	A	226	31.455	81.695	23.273	1	52.29
1711	C	PHE	A	226	32.285	82.726	22.52	1	55.03
1712	O	PHE	A	226	33.462	82.5	22.252	1	58.57
1713	CB	PHE	A	226	32.365	80.847	24.2	1	49.67
1714	CG	PHE	A	226	31.652	79.684	24.9	1	50.17
1715	CD1	PHE	A	226	30.515	79.896	25.674	1	46.15
1716	CD2	PHE	A	226	32.115	78.376	24.755	1	45.89
1717	CE1	PHE	A	226	29.857	78.834	26.279	1	47.66
1718	CE2	PHE	A	226	31.457	77.306	25.361	1	46.03
1719	CZ	PHE	A	226	30.328	77.531	26.122	1	46.99
1720	N	LYS	A	227	31.672	83.852	22.163	1	56.37
1721	CA	LYS	A	227	32.391	84.894	21.429	1	58.68
1722	C	LYS	A	227	33.043	85.866	22.4	1	60.44
1723	O	LYS	A	227	32.417	86.835	22.818	1	66.55
1724	CB	LYS	A	227	31.442	85.638	20.472	1	57.97
1725	N	GLY	A	228	34.284	85.602	22.785	1	56.04
1726	CA	GLY	A	228	34.948	86.499	23.711	1	57.52
1727	C	GLY	A	228	35.807	87.542	23.033	1	58.39
1728	O	GLY	A	228	36.307	87.299	21.943	1	60.34
1729	N	SER	A	229	36.031	88.677	23.693	1	60.8
1730	CA	SER	A	229	36.841	89.753	23.109	1	62.63
1731	C	SER	A	229	38.347	89.487	23.137	1	61.84
1732	O	SER	A	229	39.062	89.861	22.205	1	60.42
1733	CB	SER	A	229	36.518	91.112	23.754	1	65.47
1734	OG	SER	A	229	36.901	91.182	25.121	1	68.06
1735	N	ASP	A	230	38.829	88.889	24.223	1	61.24
1736	CA	ASP	A	230	40.245	88.546	24.348	1	62.31

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1737	C	ASP	A	230	40.345	87.171	25.004	1	61.21
1738	O	ASP	A	230	39.328	86.63	25.459	1	58.76
1739	CB	ASP	A	230	41.051	89.616	25.118	1	65.38
1740	CG	ASP	A	230	40.501	89.898	26.522	1	72.67
1741	OD1	ASP	A	230	39.61	90.774	26.644	1	74.17
1742	OD2	ASP	A	230	40.969	89.266	27.507	1	74.27
1743	N	HIS	A	231	41.556	86.614	25.07	1	59.36
1744	CA	HIS	A	231	41.722	85.284	25.642	1	57.51
1745	C	HIS	A	231	41.203	85.131	27.056	1	58.59
1746	O	HIS	A	231	40.656	84.084	27.408	1	57.97
1747	CB	HIS	A	231	43.158	84.802	25.535	1	56.81
1748	CG	HIS	A	231	44.141	85.592	26.341	1	58.17
1749	ND1	HIS	A	231	44.74	86.738	25.862	1	58.28
1750	CD2	HIS	A	231	44.715	85.34	27.539	1	56.46
1751	CE1	HIS	A	231	45.649	87.148	26.725	1	60.01
1752	NE2	HIS	A	231	45.655	86.318	27.754	1	58.55
1753	N	LEU	A	232	41.352	86.178	27.863	1	59.32
1754	CA	LEU	A	232	40.868	86.131	29.233	1	56.31
1755	C	LEU	A	232	39.36	86.303	29.226	1	54.89
1756	O	LEU	A	232	38.647	85.625	29.959	1	53.63
1757	CB	LEU	A	232	41.507	87.239	30.063	1	57.78
1758	CG	LEU	A	232	43.006	87.152	30.33	1	58.25
1759	CD1	LEU	A	232	43.424	88.343	31.192	1	57.87
1760	CD2	LEU	A	232	43.33	85.839	31.029	1	57.82
1761	N	ASP	A	233	38.873	87.203	28.381	1	52.94
1762	CA	ASP	A	233	37.438	87.447	28.317	1	52.88
1763	C	ASP	A	233	36.691	86.212	27.817	1	51.75
1764	O	ASP	A	233	35.496	86.041	28.086	1	50.37
1765	CB	ASP	A	233	37.137	88.65	27.428	1	50.13
1766	CG	ASP	A	233	35.659	89.001	27.41	1	53.12
1767	OD1	ASP	A	233	35.084	89.224	28.499	1	50.34
1768	OD2	ASP	A	233	35.064	89.05	26.308	1	54.43
1769	N	GLN	A	234	37.406	85.364	27.08	1	50.61
1770	CA	GLN	A	234	36.846	84.131	26.541	1	49.41
1771	C	GLN	A	234	36.494	83.222	27.717	1	49.27
1772	O	GLN	A	234	35.467	82.524	27.707	1	50.65
1773	CB	GLN	A	234	37.863	83.453	25.624	1	49.04
1774	CG	GLN	A	234	37.375	82.151	25.006	1	47.78
1775	CD	GLN	A	234	36.36	82.361	23.905	1	47.73
1776	OE1	GLN	A	234	36.505	83.262	23.083	1	47.97
1777	NE2	GLN	A	234	35.334	81.515	23.869	1	45.6
1778	N	LEU	A	235	37.33	83.261	28.749	1	45.01
1779	CA	LEU	A	235	37.07	82.47	29.927	1	46.44
1780	C	LEU	A	235	35.735	82.904	30.48	1	51.21
1781	O	LEU	A	235	34.843	82.074	30.645	1	53.59
1782	CB	LEU	A	235	38.168	82.654	30.964	1	44.69
1783	CG	LEU	A	235	39.524	82.06	30.559	1	47.12
1784	CD1	LEU	A	235	40.508	82.181	31.694	1	44.48
1785	CD2	LEU	A	235	39.365	80.586	30.187	1	44.56
1786	N	LYS	A	236	35.55	84.219	30.641	1	55.97
1787	CA	LYS	A	236	34.286	84.755	31.169	1	55.78
1788	C	LYS	A	236	33.093	84.311	30.339	1	53.9
1789	O	LYS	A	236	32.08	83.872	30.892	1	54.18
1790	CB	LYS	A	236	34.305	86.293	31.304	1	58.61
1791	CG	LYS	A	236	32.938	86.905	31.713	1	62.72
1792	CD	LYS	A	236	33.029	88.206	32.529	1	68.09

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1793	CE	LYS	A	236	33.62	89.388	31.748	1	70.68
1794	NZ	LYS	A	236	33.684	90.65	32.563	1	68.15
1795	N	GLU	A	237	33.209	84.405	29.019	1	50.88
1796	CA	GLU	A	237	32.1	83.99	28.186	1	54.56
1797	C	GLU	A	237	31.757	82.531	28.433	1	56.25
1798	O	GLU	A	237	30.587	82.191	28.598	1	57.45
1799	CB	GLU	A	237	32.373	84.243	26.7	1	56.02
1800	CG	GLU	A	237	32.014	85.656	26.21	1	56.39
1801	CD	GLU	A	237	30.623	86.1	26.643	1	55.6
1802	OE1	GLU	A	237	29.628	85.45	26.253	1	56.67
1803	OE2	GLU	A	237	30.531	87.102	27.387	1	56.02
1804	N	ILE	A	238	32.781	81.681	28.531	1	57.26
1805	CA	ILE	A	238	32.562	80.256	28.762	1	53.01
1806	C	ILE	A	238	31.946	80.045	30.121	1	52.69
1807	O	ILE	A	238	30.942	79.351	30.265	1	54.46
1808	CB	ILE	A	238	33.877	79.482	28.711	1	51.46
1809	CG1	ILE	A	238	34.454	79.532	27.292	1	45.54
1810	CG2	ILE	A	238	33.664	78.052	29.221	1	45
1811	CD1	ILE	A	238	35.9	79.119	27.202	1	40.99
1812	N	MET	A	239	32.551	80.68	31.111	1	51.8
1813	CA	MET	A	239	32.101	80.565	32.484	1	53.98
1814	C	MET	A	239	30.633	80.944	32.639	1	54.25
1815	O	MET	A	239	29.916	80.323	33.41	1	53.75
1816	CB	MET	A	239	32.951	81.457	33.39	1	58.39
1817	CG	MET	A	239	34.465	81.251	33.285	1	59.22
1818	SD	MET	A	239	35.103	79.889	34.221	1	53.8
1819	CE	MET	A	239	36.7	79.701	33.468	1	56.98
1820	N	LYS	A	240	30.178	81.953	31.902	1	53.74
1821	CA	LYS	A	240	28.789	82.378	32.015	1	53.83
1822	C	LYS	A	240	27.85	81.21	31.7	1	56.3
1823	O	LYS	A	240	26.7	81.176	32.15	1	58.97
1824	CB	LYS	A	240	28.512	83.594	31.106	1	47.67
1825	N	VAL	A	241	28.383	80.206	31.006	1	59.49
1826	CA	VAL	A	241	27.612	79.025	30.622	1	59.78
1827	C	VAL	A	241	27.917	77.786	31.451	1	59.47
1828	O	VAL	A	241	27.003	77.11	31.917	1	57.29
1829	CB	VAL	A	241	27.853	78.679	29.162	1	60.56
1830	CG1	VAL	A	241	27.066	77.44	28.772	1	62.14
1831	CG2	VAL	A	241	27.469	79.851	28.302	1	63.26
1832	N	THR	A	242	29.204	77.498	31.633	1	60.72
1833	CA	THR	A	242	29.634	76.313	32.385	1	61.22
1834	C	THR	A	242	29.802	76.57	33.867	1	61.59
1835	O	THR	A	242	30.175	75.683	34.618	1	63.32
1836	CB	THR	A	242	31.002	75.798	31.892	1	60.58
1837	OG1	THR	A	242	32.034	76.682	32.35	1	55.53
1838	CG2	THR	A	242	31.041	75.718	30.365	1	60.52
1839	N	GLY	A	243	29.542	77.789	34.294	1	62.62
1840	CA	GLY	A	243	29.74	78.092	35.691	1	62.61
1841	C	GLY	A	243	31.229	78.278	35.899	1	63.54
1842	O	GLY	A	243	32.044	77.976	35.011	1	64.34
1843	N	THR	A	244	31.587	78.805	37.061	1	63.44
1844	CA	THR	A	244	32.982	79.029	37.398	1	64.76
1845	C	THR	A	244	33.44	77.917	38.333	1	65.99
1846	O	THR	A	244	32.622	77.309	39.033	1	66.76
1847	CB	THR	A	244	33.149	80.373	38.11	1	62.43
1848	OG1	THR	A	244	32.192	80.46	39.177	1	63.24

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1849	CG2	THR	A	244	32.941	81.52	37.138	1	61.77
1850	N	PRO	A	245	34.752	77.628	38.354	1	66.25
1851	CA	PRO	A	245	35.312	76.582	39.218	1	68.52
1852	C	PRO	A	245	35.248	77.051	40.677	1	70.05
1853	O	PRO	A	245	34.965	78.224	40.948	1	71.64
1854	CB	PRO	A	245	36.782	76.521	38.775	1	65.48
1855	CG	PRO	A	245	36.797	77.145	37.444	1	65.27
1856	CD	PRO	A	245	35.815	78.257	37.563	1	65.64
1857	N	PRO	A	246	35.473	76.136	41.633	1	70.03
1858	CA	PRO	A	246	35.441	76.521	43.046	1	69.69
1859	C	PRO	A	246	36.547	77.541	43.347	1	69.33
1860	O	PRO	A	246	37.622	77.508	42.741	1	64.19
1861	CB	PRO	A	246	35.669	75.191	43.769	1	71.23
1862	CG	PRO	A	246	36.38	74.335	42.744	1	71.1
1863	CD	PRO	A	246	35.623	74.679	41.496	1	71.65
1864	N	ALA	A	247	36.258	78.451	44.275	1	70.91
1865	CA	ALA	A	247	37.192	79.503	44.646	1	71.76
1866	C	ALA	A	247	38.542	79	45.155	1	72.39
1867	O	ALA	A	247	39.572	79.646	44.922	1	71.39
1868	CB	ALA	A	247	36.55	80.434	45.659	1	74.06
1869	N	GLU	A	248	38.54	77.85	45.833	1	72.68
1870	CA	GLU	A	248	39.783	77.273	46.363	1	72.35
1871	C	GLU	A	248	40.704	76.777	45.25	1	69.53
1872	O	GLU	A	248	41.926	76.767	45.401	1	68.72
1873	CB	GLU	A	248	39.482	76.149	47.366	1	75.32
1874	CG	GLU	A	248	38.774	74.912	46.792	1	78.97
1875	CD	GLU	A	248	39.72	73.968	46.064	1	77.64
1876	OE1	GLU	A	248	40.911	73.895	46.45	1	78.83
1877	OE2	GLU	A	248	39.267	73.309	45.101	1	76.1
1878	N	PHE	A	249	40.103	76.372	44.133	1	66.74
1879	CA	PHE	A	249	40.853	75.898	42.976	1	64.3
1880	C	PHE	A	249	41.598	77.042	42.316	1	61.39
1881	O	PHE	A	249	42.794	76.949	42.054	1	60.61
1882	CB	PHE	A	249	39.916	75.243	41.941	1	65.74
1883	CG	PHE	A	249	40.554	75.039	40.585	1	65.12
1884	CD1	PHE	A	249	41.65	74.199	40.436	1	64.44
1885	CD2	PHE	A	249	40.09	75.731	39.474	1	65.16
1886	CE1	PHE	A	249	42.274	74.056	39.204	1	65.96
1887	CE2	PHE	A	249	40.709	75.594	38.235	1	65.98
1888	CZ	PHE	A	249	41.803	74.758	38.098	1	65.67
1889	N	VAL	A	250	40.87	78.116	42.035	1	58.42
1890	CA	VAL	A	250	41.451	79.271	41.381	1	58.47
1891	C	VAL	A	250	42.524	79.945	42.234	1	59.92
1892	O	VAL	A	250	43.397	80.641	41.724	1	59.56
1893	CB	VAL	A	250	40.328	80.239	40.857	1	58.77
1894	CG1	VAL	A	250	39.005	79.926	41.527	1	55.42
1895	CG2	VAL	A	250	40.716	81.713	41.014	1	57.44
1896	N	GLN	A	251	42.498	79.655	43.528	1	63.44
1897	CA	GLN	A	251	43.46	80.201	44.477	1	66.17
1898	C	GLN	A	251	44.842	79.658	44.173	1	65.76
1899	O	GLN	A	251	45.834	80.39	44.193	1	64.04
1900	CB	GLN	A	251	43.089	79.744	45.89	1	72.98
1901	CG	GLN	A	251	42.041	80.587	46.593	1	82.34
1902	CD	GLN	A	251	42.66	81.677	47.455	1	87.06
1903	OE1	GLN	A	251	43.662	82.315	47.075	1	89.37
1904	NE2	GLN	A	251	42.074	81.889	48.634	1	87.39

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1905	N	ARG	A	252	44.87	78.352	43.91	1	65.24
1906	CA	ARG	A	252	46.084	77.583	43.641	1	61.76
1907	C	ARG	A	252	46.553	77.567	42.191	1	61.07
1908	O	ARG	A	252	47.524	76.877	41.868	1	60.87
1909	CB	ARG	A	252	45.878	76.139	44.113	1	60.12
1910	CG	ARG	A	252	45.375	76.036	45.527	1	56.26
1911	CD	ARG	A	252	45.228	74.603	45.943	1	57.65
1912	NE	ARG	A	252	44.008	73.977	45.447	1	58.68
1913	CZ	ARG	A	252	43.978	72.812	44.807	1	64.29
1914	NH1	ARG	A	252	45.115	72.148	44.566	1	64.56
1915	NH2	ARG	A	252	42.807	72.262	44.484	1	63.9
1916	N	LEU	A	253	45.856	78.283	41.313	1	58.85
1917	CA	LEU	A	253	46.252	78.328	39.907	1	58.13
1918	C	LEU	A	253	47.706	78.736	39.756	1	57.02
1919	O	LEU	A	253	48.157	79.699	40.357	1	54.31
1920	CB	LEU	A	253	45.365	79.286	39.113	1	55.76
1921	CG	LEU	A	253	44.028	78.643	38.775	1	56
1922	CD1	LEU	A	253	43.136	79.649	38.066	1	55.5
1923	CD2	LEU	A	253	44.272	77.395	37.943	1	50.77
1924	N	GLN	A	254	48.424	77.955	38.963	1	58.4
1925	CA	GLN	A	254	49.83	78.175	38.69	1	60.84
1926	C	GLN	A	254	50.021	79.454	37.877	1	63.09
1927	O	GLN	A	254	50.902	80.264	38.168	1	62.24
1928	CB	GLN	A	254	50.369	76.983	37.901	1	64.22
1929	CG	GLN	A	254	51.66	76.409	38.424	1	68.16
1930	CD	GLN	A	254	52.749	77.44	38.513	1	72.41
1931	OE1	GLN	A	254	53.249	77.737	39.603	1	76.25
1932	NE2	GLN	A	254	53.118	78.014	37.368	1	72.87
1933	N	SER	A	255	49.205	79.614	36.838	1	65.92
1934	CA	SER	A	255	49.284	80.793	35.987	1	69.87
1935	C	SER	A	255	48.805	82.037	36.742	1	71.99
1936	O	SER	A	255	47.654	82.094	37.2	1	71.07
1937	CB	SER	A	255	48.452	80.6	34.715	1	68.37
1938	OG	SER	A	255	48.798	81.571	33.732	1	69.97
1939	N	ASP	A	256	49.705	83.011	36.899	1	73
1940	CA	ASP	A	256	49.374	84.255	37.59	1	73.33
1941	C	ASP	A	256	48.264	84.982	36.838	1	72.86
1942	O	ASP	A	256	47.215	85.294	37.409	1	71.63
1943	CB	ASP	A	256	50.613	85.157	37.714	1	74.14
1944	CG	ASP	A	256	51.581	84.69	38.803	1	75.83
1945	OD1	ASP	A	256	51.381	83.585	39.366	1	72.12
1946	OD2	ASP	A	256	52.539	85.444	39.1	1	75.25
1947	N	GLU	A	257	48.48	85.18	35.539	1	71.33
1948	CA	GLU	A	257	47.515	85.857	34.693	1	70.82
1949	C	GLU	A	257	46.122	85.235	34.825	1	69
1950	O	GLU	A	257	45.142	85.943	35.057	1	70.87
1951	CB	GLU	A	257	47.975	85.815	33.237	1	73.48
1952	CG	GLU	A	257	47.138	86.692	32.312	1	79.68
1953	CD	GLU	A	257	47.393	86.421	30.838	1	83.87
1954	OE1	GLU	A	257	46.896	85.392	30.329	1	87.45
1955	OE2	GLU	A	257	48.075	87.241	30.185	1	84.43
1956	N	ALA	A	258	46.047	83.912	34.746	1	64.38
1957	CA	ALA	A	258	44.773	83.22	34.848	1	61.36
1958	C	ALA	A	258	44.162	83.323	36.239	1	62.25
1959	O	ALA	A	258	42.939	83.437	36.38	1	62.23
1960	CB	ALA	A	258	44.947	81.778	34.472	1	61.51

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
1961	N	LYS	A	259	45.016	83.273	37.261	1	62.86
1962	CA	LYS	A	259	44.575	83.336	38.658	1	62.1
1963	C	LYS	A	259	43.967	84.69	38.983	1	61.36
1964	O	LYS	A	259	42.892	84.768	39.568	1	61.36
1965	CB	LYS	A	259	45.742	83.053	39.607	1	61.01
1966	CG	LYS	A	259	45.335	82.949	41.071	1	59.43
1967	CD	LYS	A	259	46.552	82.934	41.973	1	61.81
1968	CE	LYS	A	259	47.336	84.23	41.841	1	62.87
1969	NZ	LYS	A	259	48.63	84.199	42.57	1	65.85
1970	N	ASN	A	260	44.676	85.752	38.621	1	61.56
1971	CA	ASN	A	260	44.187	87.098	38.854	1	63.85
1972	C	ASN	A	260	42.846	87.277	38.131	1	62.65
1973	O	ASN	A	260	41.862	87.685	38.745	1	63.44
1974	CB	ASN	A	260	45.21	88.15	38.367	1	66.73
1975	CG	ASN	A	260	46.539	88.11	39.157	1	70.36
1976	OD1	ASN	A	260	47.609	88.416	38.61	1	69.25
1977	ND2	ASN	A	260	46.467	87.738	40.443	1	68.95
1978	N	TYR	A	261	42.785	86.905	36.854	1	60.38
1979	CA	TYR	A	261	41.549	87.056	36.098	1	59.21
1980	C	TYR	A	261	40.364	86.345	36.74	1	60.2
1981	O	TYR	A	261	39.337	86.96	37.003	1	62.83
1982	CB	TYR	A	261	41.712	86.583	34.652	1	55.63
1983	CG	TYR	A	261	40.477	86.86	33.839	1	54.34
1984	CD1	TYR	A	261	40.187	88.154	33.412	1	53.78
1985	CD2	TYR	A	261	39.541	85.855	33.585	1	51.88
1986	CE1	TYR	A	261	38.998	88.449	32.764	1	53.32
1987	CE2	TYR	A	261	38.341	86.137	32.939	1	52.07
1988	CZ	TYR	A	261	38.074	87.439	32.535	1	55.96
1989	OH	TYR	A	261	36.87	87.744	31.941	1	56.83
1990	N	MET	A	262	40.509	85.055	36.999	1	61.91
1991	CA	MET	A	262	39.44	84.268	37.614	1	67
1992	C	MET	A	262	39.025	84.771	39.016	1	70.53
1993	O	MET	A	262	37.904	84.508	39.493	1	69.52
1994	CB	MET	A	262	39.87	82.797	37.691	1	65.79
1995	CG	MET	A	262	39.973	82.113	36.351	1	61.11
1996	SD	MET	A	262	38.363	81.953	35.587	1	69.48
1997	CE	MET	A	262	37.512	80.925	36.813	1	60.57
1998	N	LYS	A	263	39.952	85.472	39.671	1	73.96
1999	CA	LYS	A	263	39.754	86.027	41.014	1	75.91
2000	C	LYS	A	263	38.761	87.179	40.918	1	78.18
2001	O	LYS	A	263	37.725	87.174	41.582	1	78.79
2002	CB	LYS	A	263	41.087	86.561	41.544	1	76.69
2003	CG	LYS	A	263	41.411	86.279	43.008	1	79.65
2004	CD	LYS	A	263	41.962	84.873	43.22	1	80.55
2005	CE	LYS	A	263	42.666	84.728	44.584	1	82.92
2006	NZ	LYS	A	263	44.035	85.351	44.641	1	83.41
2007	N	GLY	A	264	39.079	88.148	40.063	1	79.73
2008	CA	GLY	A	264	38.219	89.306	39.872	1	82.86
2009	C	GLY	A	264	36.864	88.972	39.274	1	83.39
2010	O	GLY	A	264	35.882	89.699	39.45	1	83.61
2011	N	LEU	A	265	36.808	87.854	38.57	1	84.09
2012	CA	LEU	A	265	35.577	87.408	37.946	1	85.51
2013	C	LEU	A	265	34.524	87.075	39.006	1	85.92
2014	O	LEU	A	265	34.862	86.627	40.104	1	86.1
2015	CB	LEU	A	265	35.865	86.153	37.127	1	86.17
2016	CG	LEU	A	265	34.918	85.819	35.986	1	84.25

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2017	CD1	LEU	A	265	35.147	86.837	34.89	1	85.31
2018	CD2	LEU	A	265	35.195	84.415	35.476	1	85.83
2019	N	PRO	A	266	33.237	87.34	38.706	1	86.24
2020	CA	PRO	A	266	32.13	87.055	39.627	1	85.3
2021	C	PRO	A	266	32.04	85.55	39.858	1	84.88
2022	O	PRO	A	266	32.84	84.786	39.324	1	87.31
2023	CB	PRO	A	266	30.913	87.534	38.846	1	85.43
2024	CG	PRO	A	266	31.455	88.678	38.043	1	87.16
2025	CD	PRO	A	266	32.765	88.126	37.549	1	87.36
2026	N	GLU	A	267	31.067	85.117	40.644	1	83.69
2027	CA	GLU	A	267	30.911	83.693	40.901	1	82.37
2028	C	GLU	A	267	29.679	83.245	40.13	1	79.96
2029	O	GLU	A	267	28.548	83.476	40.557	1	80.72
2030	CB	GLU	A	267	30.773	83.437	42.408	1	85.51
2031	CG	GLU	A	267	30.846	81.966	42.816	1	89.58
2032	CD	GLU	A	267	31.638	81.744	44.108	1	92.32
2033	OE1	GLU	A	267	32.873	81.566	44.028	1	90.72
2034	OE2	GLU	A	267	31.028	81.738	45.202	1	95.1
2035	N	LEU	A	268	29.912	82.646	38.965	1	77.43
2036	CA	LEU	A	268	28.836	82.182	38.086	1	74.63
2037	C	LEU	A	268	28.381	80.744	38.319	1	73.3
2038	O	LEU	A	268	29.169	79.886	38.709	1	74.73
2039	CB	LEU	A	268	29.257	82.37	36.633	1	73.36
2040	CG	LEU	A	268	29.478	83.844	36.289	1	75.38
2041	CD1	LEU	A	268	30.569	84.017	35.246	1	75.55
2042	CD2	LEU	A	268	28.162	84.464	35.838	1	76.3
2043	N	GLU	A	269	27.096	80.494	38.086	1	72.05
2044	CA	GLU	A	269	26.518	79.163	38.258	1	68.74
2045	C	GLU	A	269	26.299	78.507	36.899	1	68.69
2046	O	GLU	A	269	26.07	79.195	35.894	1	68.02
2047	CB	GLU	A	269	25.197	79.253	39.022	1	69.8
2048	N	LYS	A	270	26.365	77.177	36.877	1	67.81
2049	CA	LYS	A	270	26.187	76.399	35.651	1	66.51
2050	C	LYS	A	270	24.744	76.474	35.145	1	64.72
2051	O	LYS	A	270	23.809	76.242	35.901	1	63.39
2052	CB	LYS	A	270	26.579	74.939	35.906	1	65.95
2053	CG	LYS	A	270	27.495	74.318	34.859	1	65.03
2054	CD	LYS	A	270	26.752	73.866	33.611	1	67.47
2055	CE	LYS	A	270	25.843	72.662	33.871	1	65.62
2056	NZ	LYS	A	270	25.301	72.077	32.593	1	63.93
2057	N	LYS	A	271	24.578	76.816	33.869	1	64.97
2058	CA	LYS	A	271	23.26	76.915	33.253	1	66.39
2059	C	LYS	A	271	22.95	75.599	32.56	1	67.32
2060	O	LYS	A	271	23.857	74.886	32.149	1	66.32
2061	CB	LYS	A	271	23.218	78.07	32.236	1	64.29
2062	N	ASP	A	272	21.669	75.258	32.479	1	68.76
2063	CA	ASP	A	272	21.243	74.034	31.817	1	69.07
2064	C	ASP	A	272	21.464	74.304	30.34	1	69.46
2065	O	ASP	A	272	21.092	75.377	29.85	1	70.94
2066	CB	ASP	A	272	19.754	73.789	32.075	1	71.48
2067	CG	ASP	A	272	19.306	72.392	31.667	1	73.84
2068	OD1	ASP	A	272	19.171	72.114	30.454	1	71.55
2069	OD2	ASP	A	272	19.089	71.564	32.575	1	77.98
2070	N	PHE	A	273	22.067	73.352	29.628	1	67.27
2071	CA	PHE	A	273	22.322	73.555	28.206	1	65.52
2072	C	PHE	A	273	21.072	73.694	27.354	1	64.48

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2073	O	PHE	A	273	21.047	74.484	26.418	1	61.6
2074	CB	PHE	A	273	23.25	72.476	27.651	1	64.25
2075	CG	PHE	A	273	24.709	72.749	27.9	1	62.46
2076	CD1	PHE	A	273	25.107	73.61	28.917	1	60.94
2077	CD2	PHE	A	273	25.685	72.128	27.137	1	61.49
2078	CE1	PHE	A	273	26.451	73.841	29.174	1	61.06
2079	CE2	PHE	A	273	27.036	72.354	27.388	1	61.15
2080	CZ	PHE	A	273	27.418	73.209	28.408	1	61.2
2081	N	ALA	A	274	20.022	72.964	27.715	1	68.22
2082	CA	ALA	A	274	18.75	73.008	26.985	1	70.31
2083	C	ALA	A	274	18.172	74.422	26.963	1	71.26
2084	O	ALA	A	274	17.389	74.76	26.076	1	70.9
2085	CB	ALA	A	274	17.743	72.036	27.613	1	70.17
2086	N	SER	A	275	18.58	75.233	27.942	1	72.7
2087	CA	SER	A	275	18.137	76.62	28.082	1	75.09
2088	C	SER	A	275	18.812	77.541	27.068	1	76.67
2089	O	SER	A	275	18.351	78.658	26.835	1	77.53
2090	CB	SER	A	275	18.414	77.119	29.507	1	71.52
2091	N	ILE	A	276	19.91	77.065	26.482	1	78.33
2092	CA	ILE	A	276	20.68	77.826	25.501	1	79.35
2093	C	ILE	A	276	20.347	77.388	24.082	1	81.21
2094	O	ILE	A	276	20.114	78.219	23.201	1	82.83
2095	CB	ILE	A	276	22.197	77.612	25.695	1	78.11
2096	CG1	ILE	A	276	22.574	77.792	27.161	1	76.81
2097	CG2	ILE	A	276	22.989	78.578	24.816	1	77.7
2098	CD1	ILE	A	276	24.002	77.443	27.441	1	78.58
2099	N	LEU	A	277	20.374	76.078	23.861	1	82.38
2100	CA	LEU	A	277	20.097	75.498	22.551	1	84.58
2101	C	LEU	A	277	18.588	75.43	22.323	1	88.19
2102	O	LEU	A	277	17.954	74.398	22.58	1	88.83
2103	CB	LEU	A	277	20.715	74.104	22.471	1	82.44
2104	CG	LEU	A	277	22.094	73.954	23.123	1	78.99
2105	CD1	LEU	A	277	22.548	72.525	23.032	1	77.89
2106	CD2	LEU	A	277	23.094	74.877	22.479	1	78.9
2107	N	THR	A	278	18.037	76.533	21.809	1	91.86
2108	CA	THR	A	278	16.602	76.687	21.542	1	95.6
2109	C	THR	A	278	15.878	75.502	20.89	1	96.73
2110	O	THR	A	278	15.055	74.85	21.54	1	96.5
2111	CB	THR	A	278	16.305	77.987	20.731	1	96.74
2112	OG1	THR	A	278	17.175	78.065	19.592	1	97.74
2113	CG2	THR	A	278	16.488	79.226	21.604	1	96.8
2114	N	ASN	A	279	16.173	75.233	19.618	1	97.17
2115	CA	ASN	A	279	15.521	74.139	18.895	1	97.22
2116	C	ASN	A	279	16.34	72.842	18.716	1	95.08
2117	O	ASN	A	279	16.081	72.042	17.806	1	94.98
2118	CB	ASN	A	279	14.947	74.643	17.547	1	98.87
2119	CG	ASN	A	279	16.007	75.289	16.622	1	98.85
2120	OD1	ASN	A	279	15.748	75.51	15.433	1	97.86
2121	ND2	ASN	A	279	17.181	75.6	17.167	1	98.78
2122	N	ALA	A	280	17.294	72.621	19.617	1	91.73
2123	CA	ALA	A	280	18.14	71.431	19.582	1	88.32
2124	C	ALA	A	280	17.423	70.196	20.111	1	85.96
2125	O	ALA	A	280	16.43	70.315	20.816	1	87.39
2126	CB	ALA	A	280	19.401	71.676	20.378	1	86.22
2127	N	SER	A	281	17.929	69.011	19.783	1	83.44
2128	CA	SER	A	281	17.314	67.768	20.251	1	81.03

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2129	C	SER	A	281	17.841	67.429	21.658	1	80.89
2130	O	SER	A	281	18.879	67.962	22.088	1	80.28
2131	CB	SER	A	281	17.611	66.616	19.28	1	80.4
2132	OG	SER	A	281	18.755	65.858	19.658	1	78.93
2133	N	PRO	A	282	17.123	66.558	22.402	1	79.46
2134	CA	PRO	A	282	17.503	66.136	23.757	1	76
2135	C	PRO	A	282	18.875	65.447	23.813	1	72.47
2136	O	PRO	A	282	19.733	65.847	24.601	1	72.15
2137	CB	PRO	A	282	16.368	65.18	24.14	1	77.79
2138	CG	PRO	A	282	15.89	64.639	22.826	1	78.34
2139	CD	PRO	A	282	15.867	65.899	22	1	80.18
2140	N	LEU	A	283	19.074	64.441	22.962	1	69.58
2141	CA	LEU	A	283	20.334	63.697	22.892	1	66.84
2142	C	LEU	A	283	21.498	64.606	22.501	1	65.21
2143	O	LEU	A	283	22.634	64.415	22.951	1	62.73
2144	CB	LEU	A	283	20.214	62.581	21.857	1	67.61
2145	CG	LEU	A	283	19.279	61.417	22.157	1	67.77
2146	CD1	LEU	A	283	19.057	60.566	20.908	1	67.54
2147	CD2	LEU	A	283	19.88	60.589	23.283	1	66.72
2148	N	ALA	A	284	21.203	65.569	21.629	1	63.12
2149	CA	ALA	A	284	22.191	66.522	21.133	1	60.14
2150	C	ALA	A	284	22.663	67.359	22.286	1	59.39
2151	O	ALA	A	284	23.859	67.632	22.431	1	60.98
2152	CB	ALA	A	284	21.578	67.419	20.064	1	61.39
2153	N	VAL	A	285	21.709	67.762	23.118	1	57.13
2154	CA	VAL	A	285	22.024	68.581	24.278	1	52.53
2155	C	VAL	A	285	22.856	67.757	25.239	1	52.85
2156	O	VAL	A	285	23.844	68.241	25.796	1	54.74
2157	CB	VAL	A	285	20.761	69.083	24.952	1	46.76
2158	CG1	VAL	A	285	21.095	69.769	26.245	1	46.62
2159	CG2	VAL	A	285	20.047	70.021	24.03	1	43.24
2160	N	ASN	A	286	22.504	66.487	25.384	1	53.65
2161	CA	ASN	A	286	23.262	65.634	26.285	1	54.13
2162	C	ASN	A	286	24.699	65.505	25.803	1	52.66
2163	O	ASN	A	286	25.612	65.766	26.571	1	53.03
2164	CB	ASN	A	286	22.612	64.26	26.458	1	55.87
2165	CG	ASN	A	286	23.331	63.41	27.474	1	56.36
2166	OD1	ASN	A	286	23.119	63.548	28.674	1	59.83
2167	ND2	ASN	A	286	24.224	62.557	27.002	1	57.96
2168	N	LEU	A	287	24.9	65.17	24.529	1	51.12
2169	CA	LEU	A	287	26.254	65.045	23.99	1	52.14
2170	C	LEU	A	287	27.072	66.322	24.2	1	51.93
2171	O	LEU	A	287	28.222	66.274	24.641	1	51.31
2172	CB	LEU	A	287	26.211	64.727	22.504	1	49.83
2173	CG	LEU	A	287	27.583	64.605	21.842	1	50.21
2174	CD1	LEU	A	287	28.442	63.532	22.51	1	47.77
2175	CD2	LEU	A	287	27.382	64.329	20.366	1	51
2176	N	LEU	A	288	26.464	67.459	23.882	1	52.28
2177	CA	LEU	A	288	27.119	68.749	24.037	1	51.31
2178	C	LEU	A	288	27.546	68.951	25.478	1	52.12
2179	O	LEU	A	288	28.676	69.352	25.754	1	50.35
2180	CB	LEU	A	288	26.186	69.871	23.568	1	48.57
2181	CG	LEU	A	288	26.175	70.031	22.05	1	43.02
2182	CD1	LEU	A	288	25.19	71.084	21.626	1	45.13
2183	CD2	LEU	A	288	27.569	70.4	21.596	1	45.57
2184	N	GLU	A	289	26.64	68.613	26.391	1	56.07

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2185	CA	GLU	A	289	26.884	68.72	27.826	1	57.96
2186	C	GLU	A	289	28.117	67.876	28.195	1	57.14
2187	O	GLU	A	289	28.948	68.295	28.995	1	59.49
2188	CB	GLU	A	289	25.644	68.239	28.592	1	61.42
2189	CG	GLU	A	289	25.4	68.936	29.934	1	70.06
2190	CD	GLU	A	289	24.156	69.828	29.929	1	75.57
2191	OE1	GLU	A	289	23.07	69.36	29.504	1	79.13
2192	OE2	GLU	A	289	24.257	70.996	30.367	1	77.67
2193	N	LYS	A	290	28.254	66.711	27.565	1	57.77
2194	CA	LYS	A	290	29.382	65.814	27.813	1	56.73
2195	C	LYS	A	290	30.664	66.299	27.153	1	54.56
2196	O	LYS	A	290	31.747	65.972	27.628	1	55.32
2197	CB	LYS	A	290	29.072	64.396	27.331	1	59
2198	CG	LYS	A	290	28.246	63.563	28.289	1	65.3
2199	CD	LYS	A	290	27.831	62.249	27.636	1	70.07
2200	CE	LYS	A	290	27.253	61.264	28.642	1	72.6
2201	NZ	LYS	A	290	26.061	61.794	29.375	1	75.97
2202	N	MET	A	291	30.548	67.033	26.046	1	50.46
2203	CA	MET	A	291	31.729	67.551	25.361	1	49.47
2204	C	MET	A	291	32.207	68.879	25.947	1	48.92
2205	O	MET	A	291	33.397	69.155	25.977	1	47.63
2206	CB	MET	A	291	31.475	67.733	23.86	1	50.79
2207	CG	MET	A	291	31.118	66.472	23.107	1	51.91
2208	SD	MET	A	291	31.272	66.605	21.305	1	53.03
2209	CE	MET	A	291	29.663	67.185	20.858	1	50.33
2210	N	LEU	A	292	31.282	69.701	26.429	1	52.57
2211	CA	LEU	A	292	31.651	71.003	26.977	1	51.71
2212	C	LEU	A	292	31.808	71.099	28.483	1	52.95
2213	O	LEU	A	292	31.595	72.157	29.065	1	55.5
2214	CB	LEU	A	292	30.701	72.073	26.465	1	47.99
2215	CG	LEU	A	292	30.881	72.248	24.969	1	42.58
2216	CD1	LEU	A	292	29.864	73.233	24.449	1	43.81
2217	CD2	LEU	A	292	32.283	72.736	24.724	1	44
2218	N	VAL	A	293	32.185	69.992	29.115	1	54.34
2219	CA	VAL	A	293	32.424	69.982	30.551	1	54.23
2220	C	VAL	A	293	33.725	70.746	30.8	1	56.33
2221	O	VAL	A	293	34.662	70.668	30.009	1	59.41
2222	CB	VAL	A	293	32.518	68.562	31.078	1	53.83
2223	CG1	VAL	A	293	33.25	68.539	32.409	1	59.94
2224	CG2	VAL	A	293	31.12	68	31.248	1	55.41
2225	N	LEU	A	294	33.761	71.502	31.888	1	56.82
2226	CA	LEU	A	294	34.903	72.332	32.236	1	57.42
2227	C	LEU	A	294	36.154	71.535	32.626	1	59.44
2228	O	LEU	A	294	37.299	71.966	32.404	1	55.27
2229	CB	LEU	A	294	34.479	73.263	33.368	1	56.3
2230	CG	LEU	A	294	35.393	74.456	33.587	1	61.01
2231	CD1	LEU	A	294	35.302	75.375	32.387	1	60.96
2232	CD2	LEU	A	294	34.999	75.181	34.848	1	63.07
2233	N	ASP	A	295	35.892	70.37	33.215	1	63.78
2234	CA	ASP	A	295	36.891	69.426	33.697	1	65.51
2235	C	ASP	A	295	37.369	68.562	32.533	1	66.04
2236	O	ASP	A	295	36.697	67.605	32.145	1	66.19
2237	CB	ASP	A	295	36.239	68.552	34.785	1	70.58
2238	CG	ASP	A	295	37.219	67.586	35.466	1	75.84
2239	OD1	ASP	A	295	38.46	67.725	35.307	1	76.64
2240	OD2	ASP	A	295	36.723	66.687	36.19	1	75.05

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2241	N	ALA	A	296	38.539	68.895	31.998	1	64.2
2242	CA	ALA	A	296	39.122	68.169	30.881	1	64.21
2243	C	ALA	A	296	39.072	66.653	31.017	1	66.32
2244	O	ALA	A	296	38.827	65.952	30.035	1	68.03
2245	CB	ALA	A	296	40.551	68.617	30.666	1	66.83
2246	N	GLU	A	297	39.282	66.146	32.229	1	67.54
2247	CA	GLU	A	297	39.28	64.701	32.465	1	69.08
2248	C	GLU	A	297	37.939	63.982	32.271	1	69.12
2249	O	GLU	A	297	37.899	62.89	31.7	1	68.24
2250	CB	GLU	A	297	39.837	64.39	33.857	1	73.29
2251	CG	GLU	A	297	41.315	64.755	34.046	1	77.9
2252	CD	GLU	A	297	42.278	63.895	33.215	1	76.74
2253	OE1	GLU	A	297	42.214	62.645	33.321	1	76.29
2254	OE2	GLU	A	297	43.116	64.476	32.484	1	68.77
2255	N	GLN	A	298	36.856	64.569	32.782	1	70.3
2256	CA	GLN	A	298	35.509	63.988	32.664	1	70.51
2257	C	GLN	A	298	34.925	64.235	31.279	1	67.98
2258	O	GLN	A	298	33.889	63.681	30.916	1	67.58
2259	CB	GLN	A	298	34.557	64.59	33.712	1	77.11
2260	CG	GLN	A	298	34.963	64.386	35.18	1	84.98
2261	CD	GLN	A	298	35.069	62.916	35.57	1	89.04
2262	OE1	GLN	A	298	36.034	62.5	36.231	1	88.81
2263	NE2	GLN	A	298	34.078	62.119	35.158	1	89.92
2264	N	ARG	A	299	35.601	65.087	30.515	1	65.78
2265	CA	ARG	A	299	35.175	65.441	29.173	1	61.73
2266	C	ARG	A	299	35.263	64.218	28.264	1	61
2267	O	ARG	A	299	36.294	63.532	28.206	1	62.34
2268	CB	ARG	A	299	36.032	66.602	28.65	1	58.4
2269	CG	ARG	A	299	35.414	67.371	27.505	1	54.82
2270	CD	ARG	A	299	35.606	68.862	27.702	1	51.47
2271	NE	ARG	A	299	36.961	69.289	27.398	1	49.45
2272	CZ	ARG	A	299	37.593	70.286	28.008	1	45.18
2273	NH1	ARG	A	299	37.021	70.984	28.968	1	41.01
2274	NH2	ARG	A	299	38.811	70.586	27.647	1	41.47
2275	N	VAL	A	300	34.163	63.936	27.58	1	57.9
2276	CA	VAL	A	300	34.072	62.799	26.674	1	58.42
2277	C	VAL	A	300	35.218	62.777	25.649	1	58.99
2278	O	VAL	A	300	35.803	63.812	25.336	1	59.7
2279	CB	VAL	A	300	32.705	62.816	25.939	1	57.66
2280	CG1	VAL	A	300	32.824	63.453	24.56	1	55.44
2281	CG2	VAL	A	300	32.115	61.428	25.872	1	55.5
2282	N	THR	A	301	35.589	61.584	25.193	1	59.9
2283	CA	THR	A	301	36.648	61.461	24.193	1	58.31
2284	C	THR	A	301	35.954	61.227	22.858	1	60.17
2285	O	THR	A	301	34.751	60.924	22.817	1	58.15
2286	CB	THR	A	301	37.584	60.256	24.448	1	57.9
2287	OG1	THR	A	301	36.829	59.036	24.363	1	56.38
2288	CG2	THR	A	301	38.266	60.361	25.802	1	50.97
2289	N	ALA	A	302	36.714	61.355	21.773	1	59.12
2290	CA	ALA	A	302	36.175	61.149	20.44	1	55.83
2291	C	ALA	A	302	35.57	59.758	20.348	1	56.24
2292	O	ALA	A	302	34.484	59.596	19.803	1	58.36
2293	CB	ALA	A	302	37.251	61.325	19.409	1	55.91
2294	N	GLY	A	303	36.26	58.762	20.906	1	57.09
2295	CA	GLY	A	303	35.752	57.402	20.888	1	56.42
2296	C	GLY	A	303	34.413	57.338	21.6	1	60.07

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2297	O	GLY	A	303	33.407	56.881	21.03	1	60.46
2298	N	GLU	A	304	34.397	57.837	22.84	1	61.02
2299	CA	GLU	A	304	33.193	57.86	23.667	1	60.96
2300	C	GLU	A	304	32.113	58.67	22.965	1	60.89
2301	O	GLU	A	304	30.95	58.245	22.903	1	61.63
2302	CB	GLU	A	304	33.487	58.484	25.041	1	65.27
2303	CG	GLU	A	304	34.485	57.735	25.924	1	69.45
2304	CD	GLU	A	304	34.757	58.462	27.247	1	75.82
2305	OE1	GLU	A	304	33.801	59.023	27.833	1	78.78
2306	OE2	GLU	A	304	35.924	58.471	27.71	1	77.52
2307	N	ALA	A	305	32.513	59.826	22.425	1	58.26
2308	CA	ALA	A	305	31.609	60.724	21.709	1	54.78
2309	C	ALA	A	305	30.825	59.965	20.64	1	53.25
2310	O	ALA	A	305	29.61	60.047	20.594	1	51.95
2311	CB	ALA	A	305	32.395	61.863	21.083	1	51.09
2312	N	LEU	A	306	31.533	59.2	19.814	1	53.54
2313	CA	LEU	A	306	30.931	58.41	18.746	1	52.85
2314	C	LEU	A	306	29.978	57.358	19.285	1	57.51
2315	O	LEU	A	306	28.951	57.058	18.671	1	55.46
2316	CB	LEU	A	306	32.022	57.711	17.953	1	50.42
2317	CG	LEU	A	306	32.92	58.585	17.089	1	49.59
2318	CD1	LEU	A	306	34.102	57.793	16.604	1	43.28
2319	CD2	LEU	A	306	32.114	59.131	15.916	1	49.83
2320	N	ALA	A	307	30.339	56.788	20.433	1	62.58
2321	CA	ALA	A	307	29.533	55.755	21.091	1	63.64
2322	C	ALA	A	307	28.195	56.262	21.655	1	63.94
2323	O	ALA	A	307	27.332	55.457	22.02	1	66.89
2324	CB	ALA	A	307	30.35	55.09	22.202	1	61.54
2325	N	HIS	A	308	28.018	57.586	21.699	1	59.49
2326	CA	HIS	A	308	26.806	58.207	22.238	1	55.38
2327	C	HIS	A	308	25.512	57.913	21.459	1	56.49
2328	O	HIS	A	308	25.512	57.769	20.244	1	55.81
2329	CB	HIS	A	308	27.03	59.708	22.355	1	48.83
2330	CG	HIS	A	308	26.025	60.414	23.208	1	45.66
2331	ND1	HIS	A	308	24.826	60.892	22.713	1	43.32
2332	CD2	HIS	A	308	26.062	60.768	24.514	1	42.3
2333	CE1	HIS	A	308	24.174	61.513	23.676	1	39.82
2334	NE2	HIS	A	308	24.899	61.455	24.778	1	40.32
2335	N	PRO	A	309	24.379	57.823	22.169	1	60.56
2336	CA	PRO	A	309	23.085	57.544	21.542	1	61.17
2337	C	PRO	A	309	22.665	58.535	20.471	1	61.9
2338	O	PRO	A	309	21.673	58.306	19.78	1	64.35
2339	CB	PRO	A	309	22.127	57.592	22.728	1	61.18
2340	CG	PRO	A	309	22.961	57.081	23.847	1	63.08
2341	CD	PRO	A	309	24.244	57.833	23.639	1	61.55
2342	N	TYR	A	310	23.376	59.654	20.367	1	60.89
2343	CA	TYR	A	310	23.052	60.676	19.369	1	60.03
2344	C	TYR	A	310	23.376	60.143	17.976	1	59.78
2345	O	TYR	A	310	22.63	60.362	17.016	1	55.61
2346	CB	TYR	A	310	23.865	61.959	19.634	1	60.71
2347	CG	TYR	A	310	23.661	63.068	18.614	1	57.56
2348	CD1	TYR	A	310	22.395	63.613	18.399	1	58.7
2349	CD2	TYR	A	310	24.733	63.575	17.872	1	54.92
2350	CE1	TYR	A	310	22.193	64.642	17.471	1	57.82
2351	CE2	TYR	A	310	24.543	64.601	16.935	1	55.04
2352	CZ	TYR	A	310	23.268	65.133	16.745	1	55.99

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2353	OH	TYR	A	310	23.049	66.16	15.856	1	51.18
2354	N	PHE	A	311	24.48	59.407	17.901	1	62.46
2355	CA	PHE	A	311	24.976	58.831	16.662	1	66.25
2356	C	PHE	A	311	24.476	57.404	16.464	1	72.07
2357	O	PHE	A	311	25.114	56.616	15.757	1	75.44
2358	CB	PHE	A	311	26.508	58.854	16.681	1	62.42
2359	CG	PHE	A	311	27.094	60.23	16.884	1	60.59
2360	CD1	PHE	A	311	26.792	61.272	16.007	1	61.21
2361	CD2	PHE	A	311	27.95	60.492	17.95	1	59.64
2362	CE1	PHE	A	311	27.338	62.552	16.194	1	58.52
2363	CE2	PHE	A	311	28.5	61.77	18.143	1	58.27
2364	CZ	PHE	A	311	28.193	62.795	17.266	1	55.34
2365	N	GLU	A	312	23.319	57.097	17.056	1	75.2
2366	CA	GLU	A	312	22.697	55.767	17.002	1	77.76
2367	C	GLU	A	312	22.472	55.231	15.583	1	77.48
2368	O	GLU	A	312	22.915	54.123	15.245	1	75.56
2369	CB	GLU	A	312	21.367	55.793	17.772	1	83.58
2370	CG	GLU	A	312	20.645	54.446	17.91	1	89.04
2371	CD	GLU	A	312	19.245	54.583	18.507	1	91.58
2372	OE1	GLU	A	312	18.421	55.321	17.924	1	94.32
2373	OE2	GLU	A	312	18.962	53.952	19.549	1	91.87
2374	N	SER	A	313	21.807	56.036	14.754	1	76.34
2375	CA	SER	A	313	21.498	55.662	13.372	1	74.37
2376	C	SER	A	313	22.704	55.621	12.43	1	73.93
2377	O	SER	A	313	22.549	55.396	11.228	1	71.9
2378	CB	SER	A	313	20.431	56.601	12.798	1	72.62
2379	OG	SER	A	313	20.929	57.916	12.647	1	70.9
2380	N	LEU	A	314	23.901	55.802	12.976	1	73.98
2381	CA	LEU	A	314	25.102	55.794	12.157	1	75.64
2382	C	LEU	A	314	26.186	54.828	12.657	1	78.57
2383	O	LEU	A	314	27.044	54.404	11.874	1	78.19
2384	CB	LEU	A	314	25.672	57.218	12.071	1	74.66
2385	CG	LEU	A	314	24.779	58.387	11.625	1	71.8
2386	CD1	LEU	A	314	25.527	59.698	11.801	1	69.63
2387	CD2	LEU	A	314	24.348	58.222	10.177	1	70.16
2388	N	HIS	A	315	26.12	54.465	13.945	1	81.27
2389	CA	HIS	A	315	27.088	53.569	14.61	1	83.32
2390	C	HIS	A	315	27.419	52.221	13.922	1	84.7
2391	O	HIS	A	315	26.613	51.753	13.084	1	85.92
2392	CB	HIS	A	315	26.651	53.328	16.069	1	81.93
2393	OXT	HIS	A	315	28.491	51.636	14.23	1	82.02
2394	N	GLN	A	322	42.293	49.682	13.733	1	86.57
2395	CA	GLN	A	322	43.44	50.091	14.6	1	88.79
2396	C	GLN	A	322	44.391	51.01	13.816	1	89.57
2397	O	GLN	A	322	44.502	50.893	12.582	1	88.38
2398	CB	GLN	A	322	44.176	48.854	15.122	1	89.1
2399	N	VAL	A	323	45.078	51.914	14.527	1	88.86
2400	CA	VAL	A	323	45.981	52.874	13.872	1	88.07
2401	C	VAL	A	323	47.447	52.934	14.322	1	87.21
2402	O	VAL	A	323	47.788	52.739	15.501	1	85.22
2403	CB	VAL	A	323	45.417	54.326	13.922	1	87.12
2404	CG1	VAL	A	323	43.921	54.343	13.623	1	86.52
2405	CG2	VAL	A	323	45.701	54.951	15.255	1	86.12
2406	N	GLN	A	324	48.289	53.298	13.36	1	85.99
2407	CA	GLN	A	324	49.727	53.418	13.559	1	85.96
2408	C	GLN	A	324	50.086	54.782	14.13	1	84.87

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2409	O	GLN	A	324	49.899	55.816	13.477	1	86.2
2410	CB	GLN	A	324	50.463	53.192	12.227	1	87.87
2411	N	LYS	A	325	50.621	54.777	15.344	1	81.3
2412	CA	LYS	A	325	51.015	56.009	15.998	1	79.16
2413	C	LYS	A	325	52.109	56.733	15.228	1	77.26
2414	O	LYS	A	325	53.028	56.112	14.713	1	77.74
2415	CB	LYS	A	325	51.475	55.729	17.426	1	80.69
2416	CG	LYS	A	325	50.351	55.287	18.366	1	84.68
2417	CD	LYS	A	325	50.725	55.552	19.819	1	88.94
2418	CE	LYS	A	325	51.212	56.998	19.995	1	91.51
2419	NZ	LYS	A	325	51.477	57.37	21.416	1	91.97
2420	N	TYR	A	326	51.968	58.047	15.108	1	76.32
2421	CA	TYR	A	326	52.948	58.874	14.418	1	76.35
2422	C	TYR	A	326	54.211	58.921	15.29	1	80.86
2423	O	TYR	A	326	54.115	58.889	16.519	1	82
2424	CB	TYR	A	326	52.352	60.272	14.195	1	68.98
2425	CG	TYR	A	326	53.311	61.304	13.668	1	63.42
2426	CD1	TYR	A	326	53.667	61.346	12.329	1	65.98
2427	CD2	TYR	A	326	53.874	62.24	14.52	1	64.75
2428	CE1	TYR	A	326	54.573	62.307	11.851	1	67.91
2429	CE2	TYR	A	326	54.778	63.198	14.064	1	66.04
2430	CZ	TYR	A	326	55.126	63.23	12.733	1	67.09
2431	OH	TYR	A	326	56.029	64.183	12.307	1	66.12
2432	N	ASP	A	327	55.386	58.966	14.66	1	85.46
2433	CA	ASP	A	327	56.665	58.996	15.385	1	88.92
2434	C	ASP	A	327	57.555	60.122	14.835	1	89.81
2435	O	ASP	A	327	57.327	60.579	13.717	1	89.6
2436	CB	ASP	A	327	57.356	57.64	15.207	1	92.6
2437	CG	ASP	A	327	58.449	57.395	16.228	1	96.72
2438	OD1	ASP	A	327	58.152	57.452	17.449	1	97.04
2439	OD2	ASP	A	327	59.597	57.128	15.802	1	96.71
2440	N	ASP	A	328	58.567	60.561	15.589	1	91.43
2441	CA	ASP	A	328	59.437	61.641	15.098	1	95.64
2442	C	ASP	A	328	60.7	62.002	15.914	1	96.78
2443	O	ASP	A	328	60.964	61.456	16.994	1	94.25
2444	CB	ASP	A	328	58.594	62.915	14.876	1	98.53
2445	CG	ASP	A	328	59.321	63.985	14.058	1	99.84
2446	OD1	ASP	A	328	59.618	63.737	12.868	1	99.15
2447	OD2	ASP	A	328	59.596	65.074	14.614	1	100
2448	N	SER	A	329	61.483	62.912	15.329	1	97.59
2449	CA	SER	A	329	62.716	63.461	15.888	1	98.55
2450	C	SER	A	329	62.967	64.84	15.233	1	98.82
2451	O	SER	A	329	63.589	64.92	14.149	1	97.91
2452	CB	SER	A	329	63.911	62.5	15.681	1	98.4
2453	OG	SER	A	329	64.182	62.229	14.313	1	95.53
2454	OXT	SER	A	329	62.472	65.842	15.793	1	99.25
2455	N	ARG	A	335	66.574	73.051	17.072	1	96.21
2456	CA	ARG	A	335	67.107	73.039	15.674	1	97.17
2457	C	ARG	A	335	67.192	74.454	15.088	1	97.18
2458	O	ARG	A	335	66.399	75.327	15.442	1	96.48
2459	CB	ARG	A	335	66.235	72.14	14.791	1	95.49
2460	N	THR	A	336	68.168	74.677	14.209	1	98.59
2461	CA	THR	A	336	68.366	75.984	13.564	1	99.84
2462	C	THR	A	336	67.368	76.221	12.418	1	99.87
2463	O	THR	A	336	66.68	75.293	11.987	1	99.03
2464	CB	THR	A	336	69.833	76.154	13.014	1	100

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2465	OG1	THR	A	336	70.094	75.2	11.975	1	98.96
2466	CG2	THR	A	336	70.854	75.962	14.128	1	100
2467	N	LEU	A	337	67.282	77.466	11.94	1	100
2468	CA	LEU	A	337	66.375	77.812	10.841	1	99.62
2469	C	LEU	A	337	66.735	76.959	9.63	1	100
2470	O	LEU	A	337	65.857	76.453	8.926	1	100
2471	CB	LEU	A	337	66.479	79.303	10.497	1	97.19
2472	N	ASP	A	338	68.036	76.768	9.427	1	100
2473	CA	ASP	A	338	68.538	75.964	8.321	1	99.97
2474	C	ASP	A	338	68.368	74.459	8.529	1	100
2475	O	ASP	A	338	68.46	73.689	7.569	1	100
2476	CB	ASP	A	338	69.997	76.304	8.033	1	99.46
2477	CG	ASP	A	338	70.143	77.587	7.243	1	100
2478	OD1	ASP	A	338	69.313	78.511	7.425	1	99.14
2479	OD2	ASP	A	338	71.088	77.659	6.427	1	100
2480	N	GLU	A	339	68.156	74.04	9.779	1	100
2481	CA	GLU	A	339	67.939	72.623	10.086	1	99.87
2482	C	GLU	A	339	66.495	72.269	9.739	1	99.1
2483	O	GLU	A	339	66.23	71.212	9.162	1	100
2484	CB	GLU	A	339	68.235	72.311	11.559	1	99.85
2485	CG	GLU	A	339	69.713	72.036	11.844	1	100
2486	CD	GLU	A	339	70.015	71.802	13.32	1	100
2487	OE1	GLU	A	339	69.468	70.835	13.901	1	100
2488	OE2	GLU	A	339	70.814	72.579	13.894	1	99.8
2489	N	TRP	A	340	65.571	73.17	10.074	1	97.23
2490	CA	TRP	A	340	64.155	72.979	9.765	1	94.09
2491	C	TRP	A	340	63.972	72.993	8.252	1	93.74
2492	O	TRP	A	340	63.292	72.131	7.696	1	92.91
2493	CB	TRP	A	340	63.308	74.092	10.383	1	90.8
2494	CG	TRP	A	340	63.087	73.947	11.846	1	87.46
2495	CD1	TRP	A	340	63.553	74.769	12.83	1	86.61
2496	CD2	TRP	A	340	62.339	72.917	12.503	1	84.86
2497	NE1	TRP	A	340	63.143	74.313	14.058	1	85.54
2498	CE2	TRP	A	340	62.396	73.177	13.885	1	84.66
2499	CE3	TRP	A	340	61.628	71.798	12.056	1	83.2
2500	CZ2	TRP	A	340	61.766	72.359	14.829	1	84.88
2501	CZ3	TRP	A	340	61.002	70.984	12.996	1	83.43
2502	CH2	TRP	A	340	61.076	71.27	14.365	1	83.1
2503	N	LYS	A	341	64.609	73.97	7.605	1	92.33
2504	CA	LYS	A	341	64.564	74.15	6.156	1	90.6
2505	C	LYS	A	341	65.068	72.888	5.442	1	89.72
2506	O	LYS	A	341	64.451	72.415	4.482	1	88.1
2507	CB	LYS	A	341	65.415	75.37	5.793	1	90.99
2508	CG	LYS	A	341	65.331	75.864	4.365	1	91.86
2509	CD	LYS	A	341	66.055	77.205	4.263	1	93.95
2510	CE	LYS	A	341	66.187	77.697	2.831	1	95.81
2511	NZ	LYS	A	341	66.808	79.05	2.76	1	96.07
2512	N	ARG	A	342	66.159	72.321	5.957	1	89.21
2513	CA	ARG	A	342	66.758	71.108	5.395	1	88.95
2514	C	ARG	A	342	65.911	69.868	5.677	1	87.46
2515	O	ARG	A	342	65.649	69.071	4.772	1	87.88
2516	CB	ARG	A	342	68.181	70.91	5.932	1	89.22
2517	N	VAL	A	343	65.503	69.701	6.935	1	84.84
2518	CA	VAL	A	343	64.675	68.566	7.332	1	82.31
2519	C	VAL	A	343	63.38	68.568	6.512	1	82.44
2520	O	VAL	A	343	62.898	67.511	6.095	1	83.25

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2521	CB	VAL	A	343	64.364	68.634	8.824	1	78.29
2522	N	THR	A	344	62.854	69.766	6.251	1	80.67
2523	CA	THR	A	344	61.627	69.949	5.478	1	77.41
2524	C	THR	A	344	61.846	69.587	4.018	1	77.01
2525	O	THR	A	344	61.12	68.759	3.467	1	75.78
2526	CB	THR	A	344	61.124	71.416	5.569	1	77.39
2527	OG1	THR	A	344	60.759	71.713	6.923	1	77.62
2528	CG2	THR	A	344	59.921	71.641	4.677	1	75.64
2529	N	TYR	A	345	62.852	70.211	3.403	1	77.47
2530	CA	TYR	A	345	63.193	69.974	1.996	1	76.55
2531	C	TYR	A	345	63.248	68.477	1.699	1	74.62
2532	O	TYR	A	345	62.768	68.028	0.664	1	74.1
2533	CB	TYR	A	345	64.538	70.626	1.665	1	76.48
2534	CG	TYR	A	345	64.883	70.636	0.195	1	79.82
2535	CD1	TYR	A	345	64.058	71.276	-0.727	1	81.53
2536	CD2	TYR	A	345	66.039	70.007	-0.278	1	81.39
2537	CE1	TYR	A	345	64.369	71.29	-2.094	1	83.78
2538	CE2	TYR	A	345	66.363	70.014	-1.642	1	82.74
2539	CZ	TYR	A	345	65.521	70.658	-2.545	1	84.59
2540	OH	TYR	A	345	65.81	70.654	-3.897	1	86.28
2541	N	LYS	A	346	63.81	67.715	2.636	1	75.04
2542	CA	LYS	A	346	63.928	66.265	2.513	1	74.66
2543	C	LYS	A	346	62.549	65.592	2.472	1	74.18
2544	O	LYS	A	346	62.288	64.749	1.614	1	75.1
2545	CB	LYS	A	346	64.767	65.71	3.66	1	72.9
2546	N	GLU	A	347	61.659	65.99	3.378	1	74.17
2547	CA	GLU	A	347	60.308	65.433	3.424	1	72.66
2548	C	GLU	A	347	59.482	65.854	2.209	1	72.93
2549	O	GLU	A	347	58.482	65.223	1.896	1	74.79
2550	CB	GLU	A	347	59.591	65.826	4.72	1	70.51
2551	CG	GLU	A	347	60.099	65.119	5.985	1	72.71
2552	CD	GLU	A	347	59.707	63.633	6.07	1	76.33
2553	OE1	GLU	A	347	58.563	63.277	5.706	1	75.42
2554	OE2	GLU	A	347	60.536	62.818	6.535	1	75.05
2555	N	VAL	A	348	59.898	66.916	1.525	1	72.95
2556	CA	VAL	A	348	59.183	67.384	0.338	1	73.7
2557	C	VAL	A	348	59.567	66.529	-0.875	1	74.8
2558	O	VAL	A	348	58.71	66.081	-1.642	1	74.45
2559	CB	VAL	A	348	59.493	68.883	0.02	1	71.95
2560	CG1	VAL	A	348	58.76	69.319	-1.23	1	68.63
2561	CG2	VAL	A	348	59.088	69.769	1.183	1	70.64
2562	N	LEU	A	349	60.864	66.286	-1.025	1	75.31
2563	CA	LEU	A	349	61.366	65.506	-2.142	1	73.24
2564	C	LEU	A	349	61.069	64.018	-2.026	1	71.64
2565	O	LEU	A	349	61.005	63.323	-3.037	1	72.52
2566	CB	LEU	A	349	62.866	65.734	-2.305	1	74.06
2567	CG	LEU	A	349	63.296	67.181	-2.558	1	74.01
2568	CD1	LEU	A	349	64.79	67.214	-2.831	1	74.92
2569	CD2	LEU	A	349	62.532	67.775	-3.733	1	73.53
2570	N	SER	A	350	60.882	63.535	-0.801	1	69.25
2571	CA	SER	A	350	60.594	62.116	-0.573	1	69.89
2572	C	SER	A	350	59.115	61.741	-0.741	1	70.37
2573	O	SER	A	350	58.715	60.607	-0.471	1	68.27
2574	CB	SER	A	350	61.096	61.671	0.815	1	70.53
2575	OG	SER	A	350	60.405	62.298	1.889	1	68.02
2576	N	PHE	A	351	58.314	62.679	-1.232	1	69.89

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2577	CA	PHE	A	351	56.898	62.419	-1.396	1	69.52
2578	C	PHE	A	351	56.532	61.61	-2.624	1	70.22
2579	O	PHE	A	351	56.872	61.976	-3.748	1	69.53
2580	CB	PHE	A	351	56.113	63.721	-1.417	1	67.98
2581	CG	PHE	A	351	54.63	63.52	-1.457	1	65.98
2582	CD1	PHE	A	351	53.958	63.017	-0.349	1	68.72
2583	CD2	PHE	A	351	53.907	63.808	-2.598	1	63.74
2584	CE1	PHE	A	351	52.592	62.805	-0.384	1	65.61
2585	CE2	PHE	A	351	52.544	63.6	-2.64	1	64.05
2586	CZ	PHE	A	351	51.887	63.097	-1.533	1	64.85
2587	N	LYS	A	352	55.793	60.531	-2.395	1	70.08
2588	CA	LYS	A	352	55.334	59.674	-3.476	1	71.74
2589	C	LYS	A	352	53.814	59.789	-3.503	1	72.63
2590	O	LYS	A	352	53.152	59.52	-2.501	1	73.05
2591	CB	LYS	A	352	55.761	58.234	-3.227	1	71.17
2592	N	PRO	A	353	53.244	60.221	-4.641	1	73.37
2593	CA	PRO	A	353	51.804	60.405	-4.87	1	76.13
2594	C	PRO	A	353	50.886	59.222	-4.526	1	78.04
2595	O	PRO	A	353	51.403	58.154	-4.134	1	79.75
2596	CB	PRO	A	353	51.747	60.745	-6.355	1	76.14
2597	CG	PRO	A	353	53.007	61.522	-6.56	1	75.41
2598	CD	PRO	A	353	54.014	60.675	-5.813	1	74.92
2599	OXT	PRO	A	353	49.646	59.384	-4.641	1	78.78
2600	PRO	A	353						
2601	N	ARG	B	1008	15.392	29.317	71.275	1	83.05
2602	CA	ARG	B	1008	14.307	28.341	70.997	1	83.28
2603	C	ARG	B	1008	14.782	27.225	70.048	1	84.92
2604	O	ARG	B	1008	15.892	27.289	69.491	1	85.42
2605	CB	ARG	B	1008	13.09	29.068	70.431	1	79.92
2606	N	SER	B	1009	13.957	26.183	69.917	1	84.43
2607	CA	SER	B	1009	14.251	25.03	69.064	1	82.74
2608	C	SER	B	1009	12.961	24.248	68.825	1	81.88
2609	O	SER	B	1009	12.018	24.341	69.621	1	82.17
2610	CB	SER	B	1009	15.29	24.126	69.728	1	85.86
2611	OG	SER	B	1009	15.746	23.124	68.834	1	89.93
2612	N	GLY	B	1010	12.938	23.461	67.746	1	79.73
2613	CA	GLY	B	1010	11.755	22.687	67.393	1	75.86
2614	C	GLY	B	1010	10.933	23.446	66.363	1	74.57
2615	O	GLY	B	1010	11.497	24.194	65.55	1	74.45
2616	N	PHE	B	1011	9.612	23.255	66.377	1	71.17
2617	CA	PHE	B	1011	8.712	23.944	65.445	1	67.53
2618	C	PHE	B	1011	7.493	24.464	66.178	1	68.57
2619	O	PHE	B	1011	7.383	24.316	67.392	1	70.69
2620	CB	PHE	B	1011	8.254	23.023	64.31	1	61.94
2621	CG	PHE	B	1011	9.338	22.666	63.343	1	59.04
2622	CD1	PHE	B	1011	10.255	21.653	63.641	1	60.36
2623	CD2	PHE	B	1011	9.45	23.335	62.132	1	59.42
2624	CE1	PHE	B	1011	11.278	21.306	62.743	1	60.46
2625	CE2	PHE	B	1011	10.47	23.003	61.213	1	62.65
2626	CZ	PHE	B	1011	11.389	21.981	61.522	1	61.24
2627	N	TYR	B	1012	6.608	25.12	65.44	1	69.65
2628	CA	TYR	B	1012	5.375	25.653	65.998	1	73.68
2629	C	TYR	B	1012	4.446	26.096	64.871	1	76.63
2630	O	TYR	B	1012	4.886	26.28	63.735	1	77.42
2631	CB	TYR	B	1012	5.638	26.759	67.037	1	74.22
2632	CG	TYR	B	1012	5.747	28.185	66.54	1	76.73

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2633	CD1	TYR	B	1012	6.984	28.732	66.202	1	76.4
2634	CD2	TYR	B	1012	4.629	29.017	66.511	1	77.35
2635	CE1	TYR	B	1012	7.112	30.075	65.86	1	78.03
2636	CE2	TYR	B	1012	4.742	30.358	66.167	1	80.11
2637	CZ	TYR	B	1012	5.988	30.887	65.848	1	79.91
2638	OH	TYR	B	1012	6.108	32.231	65.556	1	79.31
2639	N	ARG	B	1013	3.16	26.244	65.18	1	79.26
2640	CA	ARG	B	1013	2.177	26.589	64.159	1	81.64
2641	C	ARG	B	1013	1.4	27.85	64.478	1	82.41
2642	O	ARG	B	1013	1.181	28.173	65.643	1	82.46
2643	CB	ARG	B	1013	1.217	25.422	63.978	1	83.6
2644	CG	ARG	B	1013	1.889	24.058	64.054	1	89.93
2645	CD	ARG	B	1013	0.806	23.013	64.153	1	95.11
2646	NE	ARG	B	1013	0.367	22.626	62.863	1	97.65
2647	CZ	ARG	B	1013	-0.628	22.871	62.023	1	98.87
2648	NH1	ARG	B	1013	-1.694	23.657	62.174	1	100
2649	NH2	ARG	B	1013	-0.45	22.207	60.898	1	97.49
2650	N	GLN	B	1014	0.971	28.553	63.433	1	84.44
2651	CA	GLN	B	1014	0.217	29.791	63.611	1	86.4
2652	C	GLN	B	1014	-0.744	30.103	62.47	1	87.23
2653	O	GLN	B	1014	-0.535	29.714	61.321	1	85.7
2654	CB	GLN	B	1014	1.175	30.982	63.798	1	85.77
2655	CG	GLN	B	1014	0.482	32.265	64.231	1	85.42
2656	CD	GLN	B	1014	1.43	33.439	64.38	1	87.14
2657	OE1	GLN	B	1014	1.093	34.568	64.013	1	84.55
2658	NE2	GLN	B	1014	2.616	33.188	64.936	1	88.89
2659	N	GLU	B	1015	-1.826	30.779	62.831	1	90.63
2660	CA	GLU	B	1015	-2.848	31.213	61.89	1	94.09
2661	C	GLU	B	1015	-2.388	32.564	61.377	1	96.22
2662	O	GLU	B	1015	-2.318	33.531	62.142	1	97.87
2663	CB	GLU	B	1015	-4.184	31.399	62.619	1	95.54
2664	CG	GLU	B	1015	-4.057	32.143	63.968	1	99.7
2665	CD	GLU	B	1015	-5.372	32.746	64.473	1	100
2666	OE1	GLU	B	1015	-6.287	31.966	64.845	1	100
2667	OE2	GLU	B	1015	-5.474	34.001	64.518	1	100
2668	N	VAL	B	1016	-2.019	32.636	60.107	1	97.88
2669	CA	VAL	B	1016	-1.588	33.919	59.565	1	99.97
2670	C	VAL	B	1016	-2.798	34.646	58.96	1	100
2671	O	VAL	B	1016	-3.478	35.414	59.659	1	100
2672	CB	VAL	B	1016	-0.418	33.757	58.571	1	100
2673	CG1	VAL	B	1016	-0.013	35.12	58.006	1	100
2674	CG2	VAL	B	1016	0.767	33.161	59.3	1	98.23
2675	N	THR	B	1017	-3.047	34.451	57.669	1	99.17
2676	CA	THR	B	1017	-4.221	35.064	57.068	1	99.53
2677	C	THR	B	1017	-5.262	33.954	57.11	1	100
2678	O	THR	B	1017	-5.856	33.693	58.166	1	100
2679	CB	THR	B	1017	-3.979	35.538	55.624	1	99.86
2680	OG1	THR	B	1017	-2.826	34.876	55.081	1	100
2681	CG2	THR	B	1017	-3.802	37.059	55.586	1	97.41
2682	N	LYS	B	1018	-5.42	33.249	55.992	1	100
2683	CA	LYS	B	1018	-6.361	32.141	55.915	1	99.37
2684	C	LYS	B	1018	-5.574	30.839	56.041	1	98.26
2685	O	LYS	B	1018	-6.108	29.802	56.441	1	99.14
2686	CB	LYS	B	1018	-7.118	32.184	54.581	1	100
2687	N	THR	B	1019	-4.277	30.932	55.766	1	96.74
2688	CA	THR	B	1019	-3.387	29.771	55.8	1	94.46

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2689	C	THR	B	1019	-2.738	29.458	57.137	1	91.56
2690	O	THR	B	1019	-2.628	30.323	58.016	1	92.58
2691	CB	THR	B	1019	-2.238	29.922	54.784	1	95.45
2692	OG1	THR	B	1019	-2.502	31.034	53.911	1	99.16
2693	CG2	THR	B	1019	-2.074	28.641	53.969	1	94.6
2694	N	ALA	B	1020	-2.271	28.213	57.252	1	87.6
2695	CA	ALA	B	1020	-1.59	27.743	58.453	1	84.33
2696	C	ALA	B	1020	-0.139	27.431	58.153	1	81.1
2697	O	ALA	B	1020	0.171	26.651	57.24	1	78.36
2698	CB	ALA	B	1020	-2.267	26.522	59.007	1	83.52
2699	N	TRP	B	1021	0.735	28.034	58.954	1	79.36
2700	CA	TRP	B	1021	2.174	27.871	58.813	1	77.91
2701	C	TRP	B	1021	2.716	27.026	59.942	1	74.81
2702	O	TRP	B	1021	2.159	27.02	61.029	1	73.4
2703	CB	TRP	B	1021	2.857	29.231	58.888	1	81.21
2704	CG	TRP	B	1021	2.419	30.198	57.877	1	83.81
2705	CD1	TRP	B	1021	1.155	30.652	57.673	1	85.5
2706	CD2	TRP	B	1021	3.259	30.917	56.977	1	86.46
2707	NE1	TRP	B	1021	1.154	31.63	56.709	1	87.55
2708	CE2	TRP	B	1021	2.436	31.809	56.263	1	88.07
2709	CE3	TRP	B	1021	4.634	30.9	56.712	1	87.08
2710	CZ2	TRP	B	1021	2.94	32.679	55.298	1	88.43
2711	CZ3	TRP	B	1021	5.136	31.765	55.754	1	88.61
2712	CH2	TRP	B	1021	4.288	32.643	55.058	1	89.09
2713	N	GLU	B	1022	3.812	26.325	59.682	1	72.48
2714	CA	GLU	B	1022	4.451	25.509	60.704	1	73.8
2715	C	GLU	B	1022	5.936	25.824	60.635	1	71.25
2716	O	GLU	B	1022	6.738	25.001	60.196	1	71.35
2717	CB	GLU	B	1022	4.206	24.007	60.474	1	79.31
2718	CG	GLU	B	1022	4.517	23.095	61.701	1	84.5
2719	CD	GLU	B	1022	4.301	21.588	61.443	1	85.91
2720	OE1	GLU	B	1022	3.614	21.221	60.456	1	85.61
2721	OE2	GLU	B	1022	4.828	20.772	62.235	1	85.16
2722	N	VAL	B	1023	6.29	27.034	61.052	1	67.98
2723	CA	VAL	B	1023	7.676	27.489	61.027	1	65.19
2724	C	VAL	B	1023	8.494	26.977	62.217	1	65.74
2725	O	VAL	B	1023	7.983	26.244	63.065	1	66.88
2726	CB	VAL	B	1023	7.712	29	61.026	1	62.43
2727	CG1	VAL	B	1023	6.959	29.513	59.825	1	61.52
2728	CG2	VAL	B	1023	7.098	29.527	62.307	1	58.2
2729	N	ARG	B	1024	9.777	27.323	62.261	1	64.48
2730	CA	ARG	B	1024	10.619	26.898	63.375	1	61.55
2731	C	ARG	B	1024	10.345	27.797	64.562	1	61.75
2732	O	ARG	B	1024	9.95	28.958	64.392	1	61.74
2733	CB	ARG	B	1024	12.091	26.978	63.02	1	60.44
2734	CG	ARG	B	1024	12.504	25.966	62.016	1	57.18
2735	CD	ARG	B	1024	13.98	26.016	61.83	1	58.85
2736	NE	ARG	B	1024	14.41	25.011	60.87	1	60.61
2737	CZ	ARG	B	1024	15.62	24.972	60.329	1	61.41
2738	NH1	ARG	B	1024	16.526	25.883	60.674	1	66.93
2739	NH2	ARG	B	1024	15.924	24.028	59.449	1	56.73
2740	N	ALA	B	1025	10.567	27.252	65.759	1	60.76
2741	CA	ALA	B	1025	10.329	27.965	67.012	1	57.56
2742	C	ALA	B	1025	11.127	29.244	67.089	1	54.88
2743	O	ALA	B	1025	10.67	30.252	67.628	1	56.15
2744	CB	ALA	B	1025	10.661	27.071	68.192	1	59.62

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2745	N	VAL	B	1026	12.311	29.197	66.499	1	52.15
2746	CA	VAL	B	1026	13.228	30.317	66.48	1	50.17
2747	C	VAL	B	1026	12.692	31.528	65.713	1	49.17
2748	O	VAL	B	1026	12.807	32.658	66.179	1	46.54
2749	CB	VAL	B	1026	14.575	29.85	65.964	1	49.05
2750	CG1	VAL	B	1026	14.742	30.139	64.484	1	48.71
2751	CG2	VAL	B	1026	15.649	30.434	66.796	1	53.91
2752	N	TYR	B	1027	12.079	31.279	64.555	1	49.98
2753	CA	TYR	B	1027	11.488	32.344	63.734	1	51.49
2754	C	TYR	B	1027	10.266	32.797	64.48	1	52.19
2755	O	TYR	B	1027	9.315	32.035	64.62	1	53.66
2756	CB	TYR	B	1027	11.121	31.845	62.326	1	43.78
2757	CG	TYR	B	1027	12.35	31.484	61.54	1	40.04
2758	CD1	TYR	B	1027	13.39	32.403	61.398	1	33.52
2759	CD2	TYR	B	1027	12.523	30.195	61.026	1	40.23
2760	CE1	TYR	B	1027	14.576	32.047	60.782	1	37.28
2761	CE2	TYR	B	1027	13.71	29.823	60.392	1	41.78
2762	CZ	TYR	B	1027	14.738	30.754	60.276	1	42.27
2763	OH	TYR	B	1027	15.928	30.4	59.666	1	40.36
2764	N	ARG	B	1028	10.301	34.036	64.954	1	53.3
2765	CA	ARG	B	1028	9.219	34.571	65.746	1	56.32
2766	C	ARG	B	1028	8.473	35.767	65.169	1	58.02
2767	O	ARG	B	1028	8.881	36.338	64.164	1	58.88
2768	CB	ARG	B	1028	9.779	34.902	67.128	1	63.3
2769	CG	ARG	B	1028	10.518	33.704	67.758	1	69.98
2770	CD	ARG	B	1028	10.844	33.91	69.234	1	78.35
2771	NE	ARG	B	1028	9.665	34.345	69.984	1	84.1
2772	CZ	ARG	B	1028	9.703	35.023	71.13	1	86.57
2773	NH1	ARG	B	1028	10.865	35.347	71.685	1	86.22
2774	NH2	ARG	B	1028	8.574	35.411	71.704	1	84.89
2775	N	ASP	B	1029	7.366	36.12	65.821	1	61.08
2776	CA	ASP	B	1029	6.467	37.216	65.434	1	60.46
2777	C	ASP	B	1029	6.184	37.324	63.937	1	61.99
2778	O	ASP	B	1029	6.596	38.29	63.29	1	64.59
2779	CB	ASP	B	1029	6.963	38.56	65.975	1	61.19
2780	CG	ASP	B	1029	5.962	39.7	65.736	1	64.61
2781	OD1	ASP	B	1029	4.752	39.427	65.602	1	66.52
2782	OD2	ASP	B	1029	6.38	40.877	65.68	1	63.58
2783	N	LEU	B	1030	5.452	36.346	63.4	1	62.42
2784	CA	LEU	B	1030	5.102	36.317	61.979	1	59.79
2785	C	LEU	B	1030	4.113	37.408	61.58	1	61.03
2786	O	LEU	B	1030	3.206	37.74	62.326	1	62.72
2787	CB	LEU	B	1030	4.546	34.951	61.588	1	53.81
2788	CG	LEU	B	1030	5.494	33.753	61.569	1	54.22
2789	CD1	LEU	B	1030	4.73	32.506	61.178	1	55.1
2790	CD2	LEU	B	1030	6.597	33.966	60.577	1	55.29
2791	N	GLN	B	1031	4.315	37.967	60.393	1	64.68
2792	CA	GLN	B	1031	3.466	39.025	59.844	1	66.39
2793	C	GLN	B	1031	3.441	38.849	58.326	1	68.35
2794	O	GLN	B	1031	4.491	38.772	57.682	1	67.74
2795	CB	GLN	B	1031	4.044	40.405	60.16	1	67.52
2796	CG	GLN	B	1031	4.037	40.788	61.622	1	69.37
2797	CD	GLN	B	1031	2.655	41.127	62.108	1	70.2
2798	OE1	GLN	B	1031	2.198	40.598	63.122	1	69.64
2799	NE2	GLN	B	1031	1.975	42.022	61.388	1	69.2
2800	N	PRO	B	1032	2.239	38.816	57.733	1	68.45

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2801	CA	PRO	B	1032	2.06	38.652	56.289	1	68.35
2802	C	PRO	B	1032	2.523	39.887	55.52	1	66.87
2803	O	PRO	B	1032	2.544	40.992	56.066	1	67.31
2804	CB	PRO	B	1032	0.549	38.485	56.171	1	69.44
2805	CG	PRO	B	1032	0.061	39.446	57.216	1	67.89
2806	CD	PRO	B	1032	0.947	39.083	58.387	1	69.43
2807	N	VAL	B	1033	2.887	39.688	54.257	1	64.21
2808	CA	VAL	B	1033	3.333	40.775	53.39	1	63.04
2809	C	VAL	B	1033	3.004	40.457	51.934	1	67.16
2810	O	VAL	B	1033	2.912	41.424	51.129	1	68.52
2811	CB	VAL	B	1033	4.853	41.025	53.497	1	60.21
2812	CG1	VAL	B	1033	5.16	41.909	54.675	1	61.04
2813	CG2	VAL	B	1033	5.615	39.705	53.595	1	57.1
2814	OXT	VAL	B	1033	2.842	39.243	51.623	1	69.07
2815	N	ALA	B	1040	2.347	32.902	49.519	1	58.98
2816	CA	ALA	B	1040	2.347	33.811	50.696	1	58.02
2817	C	ALA	B	1040	3.704	33.817	51.416	1	56.39
2818	O	ALA	B	1040	4.386	32.793	51.559	1	56.11
2819	CB	ALA	B	1040	1.208	33.469	51.658	1	56.78
2820	N	VAL	B	1041	4.089	35.015	51.826	1	53.11
2821	CA	VAL	B	1041	5.348	35.262	52.488	1	51.25
2822	C	VAL	B	1041	5.056	36.015	53.769	1	51.9
2823	O	VAL	B	1041	4.111	36.83	53.833	1	51.33
2824	CB	VAL	B	1041	6.248	36.146	51.588	1	49.54
2825	CG1	VAL	B	1041	7.51	36.559	52.307	1	49.63
2826	CG2	VAL	B	1041	6.587	35.412	50.315	1	47.38
2827	N	CYS	B	1042	5.873	35.742	54.782	1	49.82
2828	CA	CYS	B	1042	5.736	36.399	56.066	1	51.12
2829	C	CYS	B	1042	7.04	37.024	56.515	1	50.9
2830	O	CYS	B	1042	8.134	36.541	56.187	1	51.95
2831	CB	CYS	B	1042	5.278	35.402	57.135	1	54.35
2832	SG	CYS	B	1042	3.513	35.225	57.304	1	55.44
2833	N	SER	B	1043	6.913	38.093	57.285	1	49.19
2834	CA	SER	B	1043	8.067	38.754	57.837	1	49.38
2835	C	SER	B	1043	8.149	38.277	59.287	1	52.16
2836	O	SER	B	1043	7.215	38.462	60.059	1	54.98
2837	CB	SER	B	1043	7.907	40.281	57.76	1	47.15
2838	OG	SER	B	1043	6.884	40.777	58.609	1	38.5
2839	N	ALA	B	1044	9.232	37.597	59.632	1	52.48
2840	CA	ALA	B	1044	9.426	37.112	60.988	1	51.72
2841	C	ALA	B	1044	10.672	37.762	61.587	1	52.53
2842	O	ALA	B	1044	11.23	38.689	61.008	1	55.34
2843	CB	ALA	B	1044	9.585	35.623	60.963	1	52.76
2844	N	VAL	B	1045	11.077	37.299	62.766	1	50.78
2845	CA	VAL	B	1045	12.276	37.798	63.426	1	50.51
2846	C	VAL	B	1045	13.061	36.58	63.847	1	52.51
2847	O	VAL	B	1045	12.48	35.646	64.383	1	55.24
2848	CB	VAL	B	1045	11.956	38.552	64.702	1	49.88
2849	CG1	VAL	B	1045	13.252	38.976	65.38	1	46.66
2850	CG2	VAL	B	1045	11.045	39.741	64.404	1	48.94
2851	N	ASP	B	1046	14.358	36.534	63.56	1	52.69
2852	CA	ASP	B	1046	15.116	35.376	64.003	1	52.1
2853	C	ASP	B	1046	15.274	35.628	65.494	1	55.1
2854	O	ASP	B	1046	15.903	36.604	65.911	1	54.02
2855	CB	ASP	B	1046	16.473	35.29	63.327	1	50.62
2856	CG	ASP	B	1046	17.168	33.976	63.6	1	53.2

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2857	OD1	ASP	B	1046	16.811	33.305	64.59	1	55.53
2858	OD2	ASP	B	1046	18.075	33.602	62.825	1	55.04
2859	N	GLY	B	1047	14.62	34.79	66.291	1	55.42
2860	CA	GLY	B	1047	14.667	34.953	67.733	1	53.43
2861	C	GLY	B	1047	16.078	34.95	68.258	1	54.89
2862	O	GLY	B	1047	16.361	35.559	69.286	1	59.29
2863	N	ARG	B	1048	16.96	34.266	67.543	1	52.22
2864	CA	ARG	B	1048	18.352	34.175	67.926	1	54.57
2865	C	ARG	B	1048	19.189	35.457	67.767	1	55.48
2866	O	ARG	B	1048	20.173	35.646	68.488	1	57.76
2867	CB	ARG	B	1048	19.017	33.07	67.117	1	55.1
2868	CG	ARG	B	1048	18.525	31.692	67.436	1	52.83
2869	CD	ARG	B	1048	19.044	30.726	66.411	1	50.53
2870	NE	ARG	B	1048	18.397	30.965	65.126	1	52.56
2871	CZ	ARG	B	1048	18.608	30.244	64.03	1	51.67
2872	NH1	ARG	B	1048	19.461	29.227	64.049	1	53.11
2873	NH2	ARG	B	1048	17.954	30.532	62.919	1	52.77
2874	N	THR	B	1049	18.829	36.321	66.818	1	55.31
2875	CA	THR	B	1049	19.617	37.526	66.583	1	52.48
2876	C	THR	B	1049	18.921	38.858	66.674	1	53.13
2877	O	THR	B	1049	19.552	39.845	67.057	1	58.57
2878	CB	THR	B	1049	20.362	37.459	65.253	1	53.85
2879	OG1	THR	B	1049	19.424	37.397	64.171	1	54.93
2880	CG2	THR	B	1049	21.297	36.24	65.228	1	52.75
2881	N	GLY	B	1050	17.643	38.906	66.311	1	54
2882	CA	GLY	B	1050	16.889	40.154	66.385	1	52.59
2883	C	GLY	B	1050	16.698	40.799	65.023	1	53.82
2884	O	GLY	B	1050	16.094	41.88	64.901	1	51.92
2885	N	ALA	B	1051	17.2	40.103	64.004	1	50.7
2886	CA	ALA	B	1051	17.148	40.552	62.623	1	52.2
2887	C	ALA	B	1051	15.856	40.123	61.918	1	53.58
2888	O	ALA	B	1051	15.524	38.931	61.937	1	53.97
2889	CB	ALA	B	1051	18.354	39.981	61.876	1	49.63
2890	N	LYS	B	1052	15.143	41.077	61.297	1	50.05
2891	CA	LYS	B	1052	13.917	40.765	60.553	1	45.76
2892	C	LYS	B	1052	14.285	39.87	59.39	1	45.14
2893	O	LYS	B	1052	15.336	40.031	58.757	1	44.51
2894	CB	LYS	B	1052	13.199	42.012	60.035	1	44.02
2895	CG	LYS	B	1052	12.616	42.884	61.127	1	51.41
2896	CD	LYS	B	1052	11.984	44.183	60.604	1	56.7
2897	CE	LYS	B	1052	10.575	43.968	60.069	1	60.61
2898	NZ	LYS	B	1052	9.957	45.254	59.614	1	61.15
2899	N	VAL	B	1053	13.406	38.913	59.13	1	45.74
2900	CA	VAL	B	1053	13.607	37.921	58.095	1	43.54
2901	C	VAL	B	1053	12.327	37.752	57.285	1	42.33
2902	O	VAL	B	1053	11.263	38.192	57.707	1	43.53
2903	CB	VAL	B	1053	14.026	36.607	58.784	1	42.05
2904	CG1	VAL	B	1053	13.293	35.404	58.222	1	44.58
2905	CG2	VAL	B	1053	15.516	36.439	58.677	1	43.33
2906	N	ALA	B	1054	12.453	37.217	56.078	1	40.46
2907	CA	ALA	B	1054	11.287	36.955	55.24	1	41.2
2908	C	ALA	B	1054	11.143	35.444	55.09	1	43.49
2909	O	ALA	B	1054	12.115	34.738	54.746	1	38.93
2910	CB	ALA	B	1054	11.447	37.591	53.892	1	39.99
2911	N	ILE	B	1055	9.945	34.945	55.396	1	45.58
2912	CA	ILE	B	1055	9.659	33.509	55.299	1	45.26

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2913	C	ILE	B	1055	8.573	33.256	54.27	1	44.36
2914	O	ILE	B	1055	7.459	33.754	54.396	1	42.33
2915	CB	ILE	B	1055	9.195	32.914	56.649	1	47.38
2916	CG1	ILE	B	1055	10.234	33.175	57.737	1	39.2
2917	CG2	ILE	B	1055	9.017	31.386	56.522	1	47.65
2918	CD1	ILE	B	1055	9.787	32.681	59.055	1	41.28
2919	N	LYS	B	1056	8.922	32.471	53.259	1	45.93
2920	CA	LYS	B	1056	8.02	32.127	52.172	1	48.46
2921	C	LYS	B	1056	7.622	30.673	52.244	1	53.81
2922	O	LYS	B	1056	8.477	29.784	52.21	1	51.61
2923	CB	LYS	B	1056	8.721	32.349	50.829	1	52.2
2924	CG	LYS	B	1056	7.869	32.05	49.604	1	49.14
2925	CD	LYS	B	1056	8.612	32.385	48.334	1	47.25
2926	CE	LYS	B	1056	7.648	32.471	47.177	1	45.82
2927	NZ	LYS	B	1056	8.316	32.917	45.925	1	41.67
2928	N	LYS	B	1057	6.317	30.438	52.302	1	58.57
2929	CA	LYS	B	1057	5.77	29.086	52.349	1	62.42
2930	C	LYS	B	1057	5.339	28.686	50.935	1	64.09
2931	O	LYS	B	1057	4.495	29.354	50.32	1	62.73
2932	CB	LYS	B	1057	4.568	29.052	53.306	1	63.07
2933	CG	LYS	B	1057	3.743	27.763	53.313	1	63.63
2934	CD	LYS	B	1057	2.538	27.893	54.269	1	65.76
2935	CE	LYS	B	1057	1.512	26.763	54.102	1	65.42
2936	NZ	LYS	B	1057	2.111	25.406	54.277	1	65.13
2937	N	LEU	B	1058	5.981	27.655	50.393	1	67.19
2938	CA	LEU	B	1058	5.628	27.157	49.069	1	70.29
2939	C	LEU	B	1058	4.233	26.562	49.182	1	74.52
2940	O	LEU	B	1058	4.022	25.558	49.878	1	72.44
2941	CB	LEU	B	1058	6.607	26.077	48.588	1	68.22
2942	CG	LEU	B	1058	7.813	26.489	47.735	1	67.54
2943	CD1	LEU	B	1058	7.346	27.223	46.488	1	68.66
2944	CD2	LEU	B	1058	8.758	27.362	48.536	1	66.95
2945	N	TYR	B	1059	3.282	27.24	48.546	1	79.9
2946	CA	TYR	B	1059	1.879	26.844	48.534	1	84.03
2947	C	TYR	B	1059	1.556	25.525	47.821	1	83.03
2948	O	TYR	B	1059	1.497	25.483	46.584	1	83.61
2949	CB	TYR	B	1059	1.069	27.947	47.833	1	89.51
2950	CG	TYR	B	1059	-0.415	27.667	47.676	1	95.91
2951	CD1	TYR	B	1059	-1.194	27.226	48.758	1	97.58
2952	CD2	TYR	B	1059	-1.045	27.85	46.437	1	97.29
2953	CE1	TYR	B	1059	-2.562	26.976	48.605	1	100
2954	CE2	TYR	B	1059	-2.411	27.603	46.274	1	100
2955	CZ	TYR	B	1059	-3.162	27.165	47.358	1	100
2956	OH	TYR	B	1059	-4.504	26.902	47.189	1	100
2957	N	ARG	B	1060	1.363	24.463	48.608	1	81.09
2958	CA	ARG	B	1060	1.069	23.112	48.101	1	79.82
2959	C	ARG	B	1060	1.907	22.76	46.865	1	76.79
2960	O	ARG	B	1060	1.367	22.474	45.8	1	75.28
2961	CB	ARG	B	1060	-0.426	22.934	47.805	1	80.83
2962	N	PRO	B	1061	3.241	22.75	47.01	1	75.64
2963	CA	PRO	B	1061	4.187	22.449	45.932	1	75.15
2964	C	PRO	B	1061	4.029	21.104	45.246	1	76.53
2965	O	PRO	B	1061	4.451	20.938	44.1	1	75.82
2966	CB	PRO	B	1061	5.54	22.567	46.627	1	73.66
2967	CG	PRO	B	1061	5.236	22.159	48.021	1	73.69
2968	CD	PRO	B	1061	3.951	22.885	48.294	1	73.79

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
2969	N	PHE	B	1062	3.423	20.144	45.932	1	78.61
2970	CA	PHE	B	1062	3.249	18.823	45.337	1	83.23
2971	C	PHE	B	1062	1.789	18.471	45.038	1	84.85
2972	O	PHE	B	1062	1.325	17.346	45.253	1	83.78
2973	CB	PHE	B	1062	3.957	17.773	46.197	1	81.92
2974	CG	PHE	B	1062	5.388	18.114	46.472	1	78.99
2975	CD1	PHE	B	1062	6.289	18.268	45.426	1	78.21
2976	CD2	PHE	B	1062	5.813	18.38	47.764	1	79.56
2977	CE1	PHE	B	1062	7.589	18.691	45.666	1	79.26
2978	CE2	PHE	B	1062	7.113	18.803	48.015	1	79.59
2979	CZ	PHE	B	1062	8.002	18.962	46.965	1	79.58
2980	N	GLN	B	1063	1.091	19.468	44.503	1	86.52
2981	CA	GLN	B	1063	-0.303	19.356	44.126	1	87.56
2982	C	GLN	B	1063	-0.371	18.984	42.636	1	89.04
2983	O	GLN	B	1063	-1.414	18.556	42.145	1	91.08
2984	CB	GLN	B	1063	-0.997	20.697	44.371	1	87.04
2985	CG	GLN	B	1063	-2.5	20.66	44.201	1	91.31
2986	CD	GLN	B	1063	-3.11	22.043	44.065	1	92.41
2987	OE1	GLN	B	1063	-2.447	22.991	43.63	1	90.05
2988	NE2	GLN	B	1063	-4.39	22.164	44.426	1	93.3
2989	N	SER	B	1064	0.741	19.148	41.921	1	87.83
2990	CA	SER	B	1064	0.801	18.821	40.496	1	88.42
2991	C	SER	B	1064	2.241	18.622	40.054	1	88.42
2992	O	SER	B	1064	3.142	18.548	40.88	1	90.12
2993	CB	SER	B	1064	0.174	19.936	39.658	1	88.4
2994	OG	SER	B	1064	1.002	21.083	39.633	1	89.39
2995	N	GLU	B	1065	2.453	18.518	38.747	1	87.68
2996	CA	GLU	B	1065	3.798	18.351	38.216	1	87.25
2997	C	GLU	B	1065	4.353	19.729	37.875	1	85.74
2998	O	GLU	B	1065	5.564	19.964	37.937	1	84.48
2999	CB	GLU	B	1065	3.775	17.475	36.963	1	90.5
3000	CG	GLU	B	1065	5.164	17.181	36.392	1	91.77
3001	CD	GLU	B	1065	5.121	16.354	35.12	1	92.8
3002	OE1	GLU	B	1065	4.616	15.204	35.171	1	92.42
3003	OE2	GLU	B	1065	5.598	16.86	34.075	1	91.25
3004	N	LEU	B	1066	3.45	20.622	37.477	1	84.13
3005	CA	LEU	B	1066	3.814	21.987	37.131	1	82.1
3006	C	LEU	B	1066	4.241	22.689	38.412	1	81.17
3007	O	LEU	B	1066	5.235	23.415	38.421	1	82.66
3008	CB	LEU	B	1066	2.626	22.731	36.498	1	82.35
3009	CG	LEU	B	1066	2.818	24.195	36.051	1	81.61
3010	CD1	LEU	B	1066	3.698	24.249	34.803	1	80.78
3011	CD2	LEU	B	1066	1.469	24.868	35.779	1	79.54
3012	N	PHE	B	1067	3.51	22.451	39.499	1	77.92
3013	CA	PHE	B	1067	3.844	23.08	40.773	1	76.72
3014	C	PHE	B	1067	5.154	22.548	41.339	1	74.37
3015	O	PHE	B	1067	6.024	23.323	41.754	1	74.07
3016	CB	PHE	B	1067	2.705	22.913	41.783	1	77.35
3017	CG	PHE	B	1067	1.578	23.901	41.604	1	79.09
3018	CD1	PHE	B	1067	1.35	24.512	40.373	1	80.39
3019	CD2	PHE	B	1067	0.741	24.218	42.672	1	81.18
3020	CE1	PHE	B	1067	0.302	25.419	40.206	1	81.06
3021	CE2	PHE	B	1067	-0.314	25.127	42.519	1	82.12
3022	CZ	PHE	B	1067	-0.532	25.728	41.282	1	81.41
3023	N	ALA	B	1068	5.305	21.227	41.306	1	71.57
3024	CA	ALA	B	1068	6.506	20.57	41.803	1	68.96

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3025	C	ALA	B	1068	7.731	21.057	41.054	1	67.07
3026	O	ALA	B	1068	8.705	21.48	41.663	1	68.86
3027	CB	ALA	B	1068	6.377	19.076	41.668	1	68.15
3028	N	LYS	B	1069	7.658	21.03	39.73	1	66.12
3029	CA	LYS	B	1069	8.761	21.473	38.888	1	65.77
3030	C	LYS	B	1069	9.215	22.887	39.261	1	64.66
3031	O	LYS	B	1069	10.411	23.152	39.394	1	63.82
3032	CB	LYS	B	1069	8.359	21.416	37.406	1	67.34
3033	CG	LYS	B	1069	9.509	21.705	36.432	1	68.81
3034	CD	LYS	B	1069	9.098	21.528	34.972	1	71.88
3035	CE	LYS	B	1069	8.014	22.526	34.544	1	73.43
3036	NZ	LYS	B	1069	7.635	22.362	33.102	1	72.84
3037	N	ARG	B	1070	8.258	23.783	39.464	1	64.21
3038	CA	ARG	B	1070	8.581	25.156	39.81	1	64.05
3039	C	ARG	B	1070	9.233	25.236	41.181	1	63.96
3040	O	ARG	B	1070	10.281	25.857	41.341	1	63.7
3041	CB	ARG	B	1070	7.329	26.028	39.714	1	65.64
3042	CG	ARG	B	1070	6.844	26.144	38.278	1	66.55
3043	CD	ARG	B	1070	5.532	26.898	38.111	1	72.46
3044	NE	ARG	B	1070	5.225	27.036	36.683	1	76.33
3045	CZ	ARG	B	1070	4.28	27.824	36.172	1	78.89
3046	NH1	ARG	B	1070	3.511	28.564	36.969	1	77.33
3047	NH2	ARG	B	1070	4.104	27.867	34.851	1	78.07
3048	N	ALA	B	1071	8.657	24.532	42.149	1	63.83
3049	CA	ALA	B	1071	9.189	24.516	43.508	1	59.39
3050	C	ALA	B	1071	10.658	24.095	43.502	1	58.85
3051	O	ALA	B	1071	11.503	24.776	44.068	1	59.6
3052	CB	ALA	B	1071	8.38	23.579	44.354	1	55.82
3053	N	TYR	B	1072	10.957	22.981	42.842	1	58.2
3054	CA	TYR	B	1072	12.321	22.484	42.756	1	57.56
3055	C	TYR	B	1072	13.212	23.48	42.029	1	57.39
3056	O	TYR	B	1072	14.332	23.724	42.45	1	60.24
3057	CB	TYR	B	1072	12.353	21.115	42.065	1	57.31
3058	CG	TYR	B	1072	13.731	20.64	41.637	1	56.65
3059	CD1	TYR	B	1072	14.277	21.035	40.418	1	57.61
3060	CD2	TYR	B	1072	14.467	19.76	42.431	1	56.47
3061	CE1	TYR	B	1072	15.516	20.56	39.997	1	60.3
3062	CE2	TYR	B	1072	15.703	19.278	42.021	1	55.38
3063	CZ	TYR	B	1072	16.221	19.681	40.805	1	59.49
3064	OH	TYR	B	1072	17.438	19.198	40.377	1	62.12
3065	N	ARG	B	1073	12.726	24.052	40.935	1	58
3066	CA	ARG	B	1073	13.517	25.037	40.201	1	58.76
3067	C	ARG	B	1073	13.847	26.265	41.057	1	59.42
3068	O	ARG	B	1073	14.961	26.792	40.979	1	62.91
3069	CB	ARG	B	1073	12.792	25.508	38.943	1	59.19
3070	CG	ARG	B	1073	12.761	24.532	37.796	1	60.52
3071	CD	ARG	B	1073	12.644	25.34	36.533	1	61.56
3072	NE	ARG	B	1073	12.287	24.561	35.354	1	62.56
3073	CZ	ARG	B	1073	11.099	24.621	34.768	1	61.61
3074	NH1	ARG	B	1073	10.129	25.37	35.292	1	60.18
3075	NH2	ARG	B	1073	10.871	23.898	33.686	1	62.46
3076	N	GLU	B	1074	12.869	26.724	41.845	1	56.17
3077	CA	GLU	B	1074	13.026	27.886	42.719	1	53.17
3078	C	GLU	B	1074	14.043	27.609	43.828	1	53.57
3079	O	GLU	B	1074	14.913	28.436	44.111	1	53.35
3080	CB	GLU	B	1074	11.681	28.282	43.328	1	49.09

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3081	CG	GLU	B	1074	11.742	29.562	44.131	1	49.98
3082	CD	GLU	B	1074	10.37	30.109	44.511	1	54.96
3083	OE1	GLU	B	1074	9.342	29.41	44.261	1	53.01
3084	OE2	GLU	B	1074	10.331	31.243	45.06	1	46.02
3085	N	LEU	B	1075	13.917	26.456	44.475	1	52.53
3086	CA	LEU	B	1075	14.855	26.089	45.515	1	51.1
3087	C	LEU	B	1075	16.262	26.035	44.912	1	53.67
3088	O	LEU	B	1075	17.131	26.81	45.302	1	53.33
3089	CB	LEU	B	1075	14.492	24.73	46.087	1	48.59
3090	CG	LEU	B	1075	15.38	24.258	47.233	1	45.59
3091	CD1	LEU	B	1075	15.456	25.324	48.312	1	40.35
3092	CD2	LEU	B	1075	14.829	22.968	47.779	1	45.47
3093	N	ARG	B	1076	16.437	25.17	43.913	1	54.76
3094	CA	ARG	B	1076	17.708	24.96	43.222	1	58
3095	C	ARG	B	1076	18.428	26.212	42.73	1	60.08
3096	O	ARG	B	1076	19.646	26.339	42.908	1	62.77
3097	CB	ARG	B	1076	17.518	23.999	42.047	1	63.86
3098	CG	ARG	B	1076	17.595	22.527	42.417	1	68.45
3099	CD	ARG	B	1076	19.031	22.022	42.442	1	72.55
3100	NE	ARG	B	1076	19.593	21.845	41.105	1	75.26
3101	CZ	ARG	B	1076	20.833	21.427	40.858	1	76.36
3102	NH1	ARG	B	1076	21.655	21.129	41.85	1	80.23
3103	NH2	ARG	B	1076	21.255	21.304	39.614	1	78.63
3104	N	LEU	B	1077	17.705	27.108	42.063	1	57.06
3105	CA	LEU	B	1077	18.317	28.337	41.567	1	53.84
3106	C	LEU	B	1077	18.745	29.242	42.718	1	52.29
3107	O	LEU	B	1077	19.81	29.856	42.67	1	51.17
3108	CB	LEU	B	1077	17.348	29.092	40.662	1	49.81
3109	CG	LEU	B	1077	16.963	28.408	39.366	1	45.19
3110	CD1	LEU	B	1077	15.734	29.034	38.832	1	43.84
3111	CD2	LEU	B	1077	18.086	28.497	38.375	1	45.19
3112	N	LEU	B	1078	17.901	29.33	43.743	1	53.72
3113	CA	LEU	B	1078	18.19	30.165	44.911	1	53.65
3114	C	LEU	B	1078	19.388	29.623	45.674	1	53.49
3115	O	LEU	B	1078	20.222	30.386	46.152	1	54.41
3116	CB	LEU	B	1078	16.965	30.275	45.819	1	49.27
3117	CG	LEU	B	1078	15.914	31.298	45.381	1	50.2
3118	CD1	LEU	B	1078	14.734	31.297	46.33	1	47.11
3119	CD2	LEU	B	1078	16.539	32.685	45.327	1	51.38
3120	N	LYS	B	1079	19.484	28.304	45.762	1	52.88
3121	CA	LYS	B	1079	20.611	27.68	46.431	1	55.99
3122	C	LYS	B	1079	21.906	27.898	45.641	1	57.03
3123	O	LYS	B	1079	22.976	27.976	46.222	1	59.51
3124	CB	LYS	B	1079	20.366	26.186	46.631	1	53.8
3125	CG	LYS	B	1079	19.41	25.867	47.763	1	55.99
3126	CD	LYS	B	1079	19.179	24.358	47.883	1	61.83
3127	CE	LYS	B	1079	20.496	23.568	47.994	1	64.12
3128	NZ	LYS	B	1079	20.278	22.094	48.021	1	59.65
3129	N	HIS	B	1080	21.8	28.042	44.327	1	57.95
3130	CA	HIS	B	1080	22.974	28.248	43.487	1	59.32
3131	C	HIS	B	1080	23.44	29.704	43.322	1	57.63
3132	O	HIS	B	1080	24.62	30.006	43.494	1	56.73
3133	CB	HIS	B	1080	22.743	27.614	42.107	1	66
3134	CG	HIS	B	1080	23.724	28.049	41.056	1	73.25
3135	ND1	HIS	B	1080	24.875	27.344	40.777	1	76.19
3136	CD2	HIS	B	1080	23.717	29.108	40.206	1	75.77

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3137	CE1	HIS	B	1080	25.535	27.947	39.803	1	78.22
3138	NE2	HIS	B	1080	24.855	29.02	39.437	1	77.24
3139	N	MET	B	1081	22.527	30.599	42.961	1	56.25
3140	CA	MET	B	1081	22.889	31.998	42.719	1	54.99
3141	C	MET	B	1081	23.491	32.695	43.932	1	52.29
3142	O	MET	B	1081	23.175	32.346	45.053	1	54.04
3143	CB	MET	B	1081	21.665	32.797	42.229	1	57.51
3144	CG	MET	B	1081	20.986	32.286	40.948	1	54.18
3145	SD	MET	B	1081	19.476	33.24	40.589	1	51.93
3146	CE	MET	B	1081	18.557	32.93	42.11	1	45.64
3147	N	ARG	B	1082	24.383	33.652	43.69	1	50.01
3148	CA	ARG	B	1082	25.007	34.445	44.756	1	50.78
3149	C	ARG	B	1082	25.377	35.835	44.211	1	49.52
3150	O	ARG	B	1082	26.421	35.995	43.554	1	50.33
3151	CB	ARG	B	1082	26.251	33.733	45.318	1	50.93
3152	N	HIS	B	1083	24.51	36.82	44.473	1	46.01
3153	CA	HIS	B	1083	24.709	38.19	43.998	1	44.84
3154	C	HIS	B	1083	24.067	39.236	44.89	1	46.37
3155	O	HIS	B	1083	22.943	39.071	45.349	1	49.77
3156	CB	HIS	B	1083	24.162	38.346	42.579	1	46.72
3157	CG	HIS	B	1083	24.558	39.632	41.935	1	46.28
3158	ND1	HIS	B	1083	23.946	40.833	42.228	1	43.36
3159	CD2	HIS	B	1083	25.563	39.92	41.072	1	43.95
3160	CE1	HIS	B	1083	24.558	41.805	41.578	1	42.91
3161	NE2	HIS	B	1083	25.543	41.28	40.872	1	45.89
3162	N	GLU	B	1084	24.751	40.363	45.047	1	49.97
3163	CA	GLU	B	1084	24.298	41.473	45.894	1	50.68
3164	C	GLU	B	1084	22.89	41.971	45.522	1	50.28
3165	O	GLU	B	1084	22.216	42.638	46.317	1	51.66
3166	CB	GLU	B	1084	25.327	42.627	45.797	1	55.77
3167	CG	GLU	B	1084	25.246	43.712	46.896	1	71.29
3168	CD	GLU	B	1084	25.737	43.254	48.305	1	80.4
3169	OE1	GLU	B	1084	26.976	43.217	48.538	1	81.58
3170	OE2	GLU	B	1084	24.884	42.969	49.191	1	82.45
3171	N	ASN	B	1085	22.436	41.624	44.32	1	48.85
3172	CA	ASN	B	1085	21.137	42.069	43.832	1	46.27
3173	C	ASN	B	1085	20.153	40.942	43.543	1	44.89
3174	O	ASN	B	1085	19.226	41.106	42.783	1	44.96
3175	CB	ASN	B	1085	21.336	42.918	42.586	1	45.28
3176	CG	ASN	B	1085	22.155	44.166	42.858	1	47.36
3177	OD1	ASN	B	1085	23.26	44.341	42.328	1	44.25
3178	ND2	ASN	B	1085	21.617	45.041	43.692	1	49.42
3179	N	VAL	B	1086	20.391	39.777	44.115	1	45.32
3180	CA	VAL	B	1086	19.506	38.647	43.923	1	43.24
3181	C	VAL	B	1086	19.281	38.086	45.318	1	46.01
3182	O	VAL	B	1086	20.244	37.819	46.058	1	49.62
3183	CB	VAL	B	1086	20.142	37.578	43.03	1	43.45
3184	CG1	VAL	B	1086	19.178	36.392	42.831	1	38.77
3185	CG2	VAL	B	1086	20.535	38.19	41.693	1	43.89
3186	N	ILE	B	1087	18.016	37.944	45.696	1	43.02
3187	CA	ILE	B	1087	17.679	37.43	47.011	1	40.27
3188	C	ILE	B	1087	18.387	36.117	47.334	1	40.11
3189	O	ILE	B	1087	18.63	35.272	46.455	1	37.82
3190	CB	ILE	B	1087	16.174	37.256	47.178	1	40.31
3191	CG1	ILE	B	1087	15.841	37.285	48.66	1	38.04
3192	CG2	ILE	B	1087	15.695	35.979	46.499	1	36.21

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3193	CD1	ILE	B	1087	16.224	38.594	49.322	1	37.07
3194	N	GLY	B	1088	18.699	35.936	48.609	1	39
3195	CA	GLY	B	1088	19.407	34.736	49.001	1	39.21
3196	C	GLY	B	1088	18.76	33.982	50.121	1	40.6
3197	O	GLY	B	1088	17.953	34.518	50.887	1	41.48
3198	N	LEU	B	1089	19.119	32.712	50.204	1	41.27
3199	CA	LEU	B	1089	18.591	31.85	51.239	1	42.74
3200	C	LEU	B	1089	19.419	31.941	52.509	1	42.21
3201	O	LEU	B	1089	20.651	31.985	52.452	1	40.32
3202	CB	LEU	B	1089	18.573	30.4	50.737	1	41.24
3203	CG	LEU	B	1089	17.256	29.862	50.183	1	37.8
3204	CD1	LEU	B	1089	16.179	30.941	50.135	1	31.91
3205	CD2	LEU	B	1089	17.508	29.277	48.82	1	36.34
3206	N	LEU	B	1090	18.73	32.045	53.64	1	41.39
3207	CA	LEU	B	1090	19.383	32.057	54.941	1	45.74
3208	C	LEU	B	1090	19.122	30.688	55.582	1	51.8
3209	O	LEU	B	1090	19.933	30.175	56.362	1	54.91
3210	CB	LEU	B	1090	18.782	33.114	55.85	1	41.25
3211	CG	LEU	B	1090	19.111	34.582	55.603	1	43.4
3212	CD1	LEU	B	1090	18.361	35.428	56.599	1	40.33
3213	CD2	LEU	B	1090	20.607	34.836	55.742	1	44.24
3214	N	ASP	B	1091	17.988	30.097	55.216	1	54.86
3215	CA	ASP	B	1091	17.56	28.818	55.755	1	56.17
3216	C	ASP	B	1091	16.404	28.346	54.886	1	58.98
3217	O	ASP	B	1091	15.781	29.139	54.174	1	58.18
3218	CB	ASP	B	1091	17.084	29.038	57.212	1	55.2
3219	CG	ASP	B	1091	16.659	27.744	57.944	1	50.83
3220	OD1	ASP	B	1091	17.182	26.645	57.654	1	48.39
3221	OD2	ASP	B	1091	15.817	27.859	58.867	1	48.11
3222	N	VAL	B	1092	16.198	27.035	54.889	1	60.54
3223	CA	VAL	B	1092	15.117	26.391	54.171	1	61.64
3224	C	VAL	B	1092	14.803	25.186	55.043	1	61.8
3225	O	VAL	B	1092	15.709	24.484	55.506	1	60.49
3226	CB	VAL	B	1092	15.523	25.948	52.746	1	63.63
3227	CG1	VAL	B	1092	16.766	25.13	52.789	1	64.29
3228	CG2	VAL	B	1092	14.412	25.119	52.11	1	64.21
3229	N	PHE	B	1093	13.522	24.959	55.291	1	62.04
3230	CA	PHE	B	1093	13.134	23.852	56.141	1	62.29
3231	C	PHE	B	1093	11.785	23.268	55.813	1	63.71
3232	O	PHE	B	1093	11.03	23.817	55.021	1	66.24
3233	CB	PHE	B	1093	13.116	24.324	57.593	1	59.66
3234	CG	PHE	B	1093	12.083	25.382	57.882	1	55.63
3235	CD1	PHE	B	1093	10.784	25.026	58.25	1	53.36
3236	CD2	PHE	B	1093	12.416	26.734	57.824	1	54.21
3237	CE1	PHE	B	1093	9.827	26.011	58.562	1	52.77
3238	CE2	PHE	B	1093	11.467	27.726	58.135	1	50.11
3239	CZ	PHE	B	1093	10.174	27.363	58.505	1	49.43
3240	N	THR	B	1094	11.485	22.161	56.477	1	66.12
3241	CA	THR	B	1094	10.21	21.475	56.339	1	67.21
3242	C	THR	B	1094	9.905	20.799	57.671	1	69
3243	O	THR	B	1094	10.739	20.079	58.229	1	67.3
3244	CB	THR	B	1094	10.206	20.421	55.204	1	67.83
3245	OG1	THR	B	1094	8.954	19.723	55.214	1	64.79
3246	CG2	THR	B	1094	11.35	19.422	55.36	1	66.66
3247	N	PRO	B	1095	8.723	21.08	58.229	1	69.99
3248	CA	PRO	B	1095	8.275	20.519	59.497	1	72.97

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3249	C	PRO	B	1095	7.784	19.079	59.333	1	77.44
3250	O	PRO	B	1095	6.995	18.58	60.139	1	79.83
3251	CB	PRO	B	1095	7.151	21.463	59.882	1	70.67
3252	CG	PRO	B	1095	6.537	21.771	58.577	1	70.21
3253	CD	PRO	B	1095	7.732	22.032	57.703	1	70.12
3254	N	ASP	B	1096	8.23	18.442	58.257	1	80.58
3255	CA	ASP	B	1096	7.876	17.064	57.952	1	84.96
3256	C	ASP	B	1096	9.146	16.236	58.15	1	88.49
3257	O	ASP	B	1096	10.153	16.423	57.453	1	88.53
3258	CB	ASP	B	1096	7.359	16.953	56.513	1	86.44
3259	CG	ASP	B	1096	6.175	17.893	56.228	1	88.55
3260	OD1	ASP	B	1096	5.37	18.178	57.146	1	88.77
3261	OD2	ASP	B	1096	6.048	18.35	55.07	1	88.75
3262	N	GLU	B	1097	9.089	15.332	59.124	1	92.02
3263	CA	GLU	B	1097	10.221	14.488	59.489	1	93.95
3264	C	GLU	B	1097	10.638	13.402	58.502	1	94.65
3265	O	GLU	B	1097	11.8	12.988	58.5	1	94.52
3266	CB	GLU	B	1097	9.973	13.892	60.874	1	95.63
3267	CG	GLU	B	1097	9.85	14.959	61.969	1	98.55
3268	CD	GLU	B	1097	9.248	14.44	63.272	1	99.67
3269	OE1	GLU	B	1097	9.588	13.307	63.69	1	100
3270	OE2	GLU	B	1097	8.437	15.177	63.88	1	97.51
3271	N	THR	B	1098	9.708	12.957	57.656	1	95.51
3272	CA	THR	B	1098	10	11.904	56.675	1	97.78
3273	C	THR	B	1098	9.549	12.247	55.253	1	97.73
3274	O	THR	B	1098	8.594	12.995	55.066	1	98.25
3275	CB	THR	B	1098	9.321	10.565	57.065	1	99.16
3276	OG1	THR	B	1098	7.899	10.742	57.109	1	99.02
3277	CG2	THR	B	1098	9.817	10.069	58.425	1	99.67
3278	N	LEU	B	1099	10.214	11.659	54.257	1	98.25
3279	CA	LEU	B	1099	9.871	11.887	52.85	1	98.51
3280	C	LEU	B	1099	8.448	11.445	52.546	1	98.29
3281	O	LEU	B	1099	7.782	12.022	51.689	1	98.53
3282	CB	LEU	B	1099	10.845	11.144	51.927	1	98.49
3283	CG	LEU	B	1099	10.488	11.023	50.436	1	98.62
3284	CD1	LEU	B	1099	10.1	12.371	49.846	1	97.83
3285	CD2	LEU	B	1099	11.664	10.422	49.67	1	99.42
3286	N	ASP	B	1100	7.994	10.418	53.259	1	99.35
3287	CA	ASP	B	1100	6.656	9.874	53.084	1	99.24
3288	C	ASP	B	1100	5.561	10.946	53.226	1	98.81
3289	O	ASP	B	1100	4.741	11.109	52.315	1	99.71
3290	CB	ASP	B	1100	6.426	8.71	54.058	1	98.7
3291	N	ASP	B	1101	5.555	11.692	54.334	1	97.21
3292	CA	ASP	B	1101	4.537	12.732	54.522	1	95.45
3293	C	ASP	B	1101	4.998	14.166	54.253	1	92.22
3294	O	ASP	B	1101	4.298	15.12	54.579	1	92.05
3295	CB	ASP	B	1101	3.813	12.604	55.882	1	98.04
3296	CG	ASP	B	1101	4.762	12.55	57.072	1	99.4
3297	OD1	ASP	B	1101	5.215	11.44	57.434	1	97.84
3298	OD2	ASP	B	1101	5.014	13.616	57.677	1	100
3299	N	PHE	B	1102	6.15	14.293	53.596	1	89.67
3300	CA	PHE	B	1102	6.745	15.583	53.22	1	85.73
3301	C	PHE	B	1102	5.831	16.283	52.232	1	83.04
3302	O	PHE	B	1102	5.894	16.009	51.039	1	84.56
3303	CB	PHE	B	1102	8.114	15.331	52.566	1	86.09
3304	CG	PHE	B	1102	8.684	16.513	51.821	1	84.91

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3305	CD1	PHE	B	1102	8.796	17.761	52.424	1	85.67
3306	CD2	PHE	B	1102	9.162	16.353	50.526	1	84.73
3307	CE1	PHE	B	1102	9.385	18.829	51.748	1	85.4
3308	CE2	PHE	B	1102	9.752	17.413	49.843	1	85.63
3309	CZ	PHE	B	1102	9.865	18.653	50.455	1	85.2
3310	N	THR	B	1103	4.975	17.174	52.72	1	78.84
3311	CA	THR	B	1103	4.061	17.874	51.831	1	77.63
3312	C	THR	B	1103	4.524	19.267	51.405	1	76.47
3313	O	THR	B	1103	4.256	19.693	50.278	1	76.17
3314	CB	THR	B	1103	2.658	17.979	52.426	1	78.02
3315	OG1	THR	B	1103	2.697	18.793	53.603	1	81.65
3316	CG2	THR	B	1103	2.127	16.597	52.776	1	79.08
3317	N	ASP	B	1104	5.228	19.972	52.285	1	75.04
3318	CA	ASP	B	1104	5.695	21.317	51.952	1	73.27
3319	C	ASP	B	1104	7.006	21.753	52.587	1	68.42
3320	O	ASP	B	1104	7.606	21.019	53.364	1	67.69
3321	CB	ASP	B	1104	4.607	22.361	52.246	1	76.28
3322	CG	ASP	B	1104	3.916	22.14	53.571	1	78.1
3323	OD1	ASP	B	1104	4.583	21.778	54.563	1	81.19
3324	OD2	ASP	B	1104	2.689	22.334	53.612	1	80.9
3325	N	PHE	B	1105	7.456	22.947	52.212	1	63.56
3326	CA	PHE	B	1105	8.685	23.499	52.742	1	60.34
3327	C	PHE	B	1105	8.701	25.006	52.698	1	58.3
3328	O	PHE	B	1105	8.029	25.619	51.873	1	58.86
3329	CB	PHE	B	1105	9.908	22.931	52.024	1	59.78
3330	CG	PHE	B	1105	10.025	23.334	50.592	1	58.24
3331	CD1	PHE	B	1105	9.211	22.762	49.629	1	57.99
3332	CD2	PHE	B	1105	11.003	24.242	50.195	1	60.55
3333	CE1	PHE	B	1105	9.371	23.082	48.282	1	60.21
3334	CE2	PHE	B	1105	11.176	24.572	48.86	1	60.36
3335	CZ	PHE	B	1105	10.36	23.988	47.897	1	62.76
3336	N	TYR	B	1106	9.49	25.592	53.594	1	56.86
3337	CA	TYR	B	1106	9.617	27.041	53.713	1	54.84
3338	C	TYR	B	1106	10.991	27.583	53.327	1	54.24
3339	O	TYR	B	1106	12.019	26.948	53.568	1	56.01
3340	CB	TYR	B	1106	9.293	27.468	55.135	1	52.86
3341	CG	TYR	B	1106	7.904	27.082	55.615	1	55.79
3342	CD1	TYR	B	1106	7.517	25.738	55.739	1	56.11
3343	CD2	TYR	B	1106	6.989	28.061	55.977	1	54.96
3344	CE1	TYR	B	1106	6.255	25.392	56.216	1	55.56
3345	CE2	TYR	B	1106	5.73	27.729	56.451	1	59.19
3346	CZ	TYR	B	1106	5.363	26.398	56.571	1	60.07
3347	OH	TYR	B	1106	4.1	26.101	57.053	1	63.38
3348	N	LEU	B	1107	10.992	28.757	52.698	1	52.76
3349	CA	LEU	B	1107	12.227	29.418	52.273	1	47.82
3350	C	LEU	B	1107	12.437	30.64	53.15	1	44.87
3351	O	LEU	B	1107	11.497	31.41	53.398	1	45.31
3352	CB	LEU	B	1107	12.139	29.867	50.814	1	42.99
3353	CG	LEU	B	1107	12.135	28.875	49.658	1	40.78
3354	CD1	LEU	B	1107	12.253	29.679	48.375	1	37.09
3355	CD2	LEU	B	1107	13.288	27.887	49.757	1	37.49
3356	N	VAL	B	1108	13.666	30.819	53.619	1	43.23
3357	CA	VAL	B	1108	13.977	31.951	54.488	1	44.7
3358	C	VAL	B	1108	15	32.877	53.856	1	45
3359	O	VAL	B	1108	16.108	32.455	53.493	1	48.26
3360	CB	VAL	B	1108	14.491	31.492	55.88	1	42.36

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3361	CG1	VAL	B	1108	14.5	32.645	56.832	1	41.98
3362	CG2	VAL	B	1108	13.591	30.414	56.455	1	44.81
3363	N	MET	B	1109	14.593	34.128	53.667	1	44.32
3364	CA	MET	B	1109	15.462	35.143	53.088	1	44.35
3365	C	MET	B	1109	15.452	36.339	54.011	1	43.05
3366	O	MET	B	1109	14.554	36.492	54.837	1	46.87
3367	CB	MET	B	1109	14.958	35.596	51.717	1	45.3
3368	CG	MET	B	1109	14.765	34.5	50.703	1	50.96
3369	SD	MET	B	1109	13.017	34.213	50.488	1	64.31
3370	CE	MET	B	1109	12.485	35.892	49.997	1	45.61
3371	N	PRO	B	1110	16.466	37.202	53.906	1	40.77
3372	CA	PRO	B	1110	16.552	38.395	54.741	1	37.5
3373	C	PRO	B	1110	15.422	39.349	54.405	1	39.62
3374	O	PRO	B	1110	15.012	39.445	53.26	1	42.95
3375	CB	PRO	B	1110	17.886	38.976	54.331	1	36.57
3376	CG	PRO	B	1110	18.092	38.474	52.981	1	32.86
3377	CD	PRO	B	1110	17.658	37.08	53.061	1	37.59
3378	N	PHE	B	1111	14.862	40.019	55.394	1	43.29
3379	CA	PHE	B	1111	13.776	40.943	55.088	1	46.86
3380	C	PHE	B	1111	14.384	42.117	54.337	1	49.91
3381	O	PHE	B	1111	15.36	42.713	54.791	1	52.95
3382	CB	PHE	B	1111	13.104	41.412	56.352	1	44.83
3383	CG	PHE	B	1111	11.964	42.337	56.118	1	46.7
3384	CD1	PHE	B	1111	10.736	41.841	55.727	1	47.93
3385	CD2	PHE	B	1111	12.091	43.702	56.371	1	50.78
3386	CE1	PHE	B	1111	9.627	42.685	55.594	1	46.11
3387	CE2	PHE	B	1111	10.989	44.555	56.242	1	53.95
3388	CZ	PHE	B	1111	9.754	44.036	55.853	1	51.1
3389	N	MET	B	1112	13.825	42.423	53.177	1	49.74
3390	CA	MET	B	1112	14.344	43.496	52.362	1	49.77
3391	C	MET	B	1112	13.54	44.777	52.312	1	49.4
3392	O	MET	B	1112	13.663	45.514	51.353	1	54.65
3393	CB	MET	B	1112	14.572	42.996	50.948	1	51.73
3394	CG	MET	B	1112	15.907	42.356	50.734	1	57.71
3395	SD	MET	B	1112	17.232	43.558	50.992	1	59.73
3396	CE	MET	B	1112	16.8	44.823	49.883	1	59.1
3397	N	GLY	B	1113	12.732	45.057	53.324	1	47.34
3398	CA	GLY	B	1113	11.977	46.293	53.316	1	47.17
3399	C	GLY	B	1113	10.563	46.198	52.79	1	50.34
3400	O	GLY	B	1113	9.623	46.08	53.583	1	56.84
3401	N	THR	B	1114	10.399	46.403	51.483	1	47.67
3402	CA	THR	B	1114	9.106	46.319	50.788	1	48.71
3403	C	THR	B	1114	9.448	46.065	49.338	1	48.49
3404	O	THR	B	1114	10.618	46.121	48.968	1	52.16
3405	CB	THR	B	1114	8.248	47.621	50.83	1	50.25
3406	OG1	THR	B	1114	8.99	48.715	50.285	1	52.88
3407	CG2	THR	B	1114	7.793	47.951	52.235	1	53.9
3408	N	ASP	B	1115	8.445	45.775	48.519	1	46.96
3409	CA	ASP	B	1115	8.681	45.519	47.108	1	46.31
3410	C	ASP	B	1115	8.426	46.811	46.352	1	45.48
3411	O	ASP	B	1115	7.636	47.63	46.796	1	44.32
3412	CB	ASP	B	1115	7.774	44.395	46.603	1	48.02
3413	CG	ASP	B	1115	6.303	44.719	46.757	1	51
3414	OD1	ASP	B	1115	5.8	45.623	46.051	1	49.24
3415	OD2	ASP	B	1115	5.649	44.078	47.602	1	54.92
3416	N	LEU	B	1116	9.063	46.961	45.193	1	44.79

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3417	CA	LEU	B	1116	8.947	48.17	44.386	1	47.63
3418	C	LEU	B	1116	7.509	48.584	44.107	1	50.96
3419	O	LEU	B	1116	7.202	49.78	44.044	1	48.13
3420	CB	LEU	B	1116	9.705	48.007	43.066	1	48.87
3421	CG	LEU	B	1116	10.009	49.289	42.28	1	47.8
3422	CD1	LEU	B	1116	10.892	50.213	43.113	1	46.89
3423	CD2	LEU	B	1116	10.671	48.956	40.952	1	43.9
3424	N	GLY	B	1117	6.638	47.588	43.943	1	51.88
3425	CA	GLY	B	1117	5.238	47.857	43.676	1	51.75
3426	C	GLY	B	1117	4.587	48.722	44.734	1	52.41
3427	O	GLY	B	1117	3.961	49.724	44.403	1	51.13
3428	N	LYS	B	1118	4.732	48.321	45.997	1	55.29
3429	CA	LYS	B	1118	4.166	49.051	47.128	1	55.85
3430	C	LYS	B	1118	4.881	50.372	47.276	1	56.27
3431	O	LYS	B	1118	4.265	51.391	47.521	1	56.48
3432	CB	LYS	B	1118	4.318	48.256	48.434	1	59.36
3433	CG	LYS	B	1118	3.565	46.924	48.476	1	65.6
3434	CD	LYS	B	1118	3.613	46.283	49.873	1	72.16
3435	CE	LYS	B	1118	3.192	44.789	49.872	1	77.1
3436	NZ	LYS	B	1118	1.815	44.51	49.352	1	78.56
3437	N	LEU	B	1119	6.195	50.351	47.114	1	57.8
3438	CA	LEU	B	1119	6.986	51.562	47.242	1	58.21
3439	C	LEU	B	1119	6.492	52.65	46.297	1	58.79
3440	O	LEU	B	1119	6.452	53.811	46.667	1	61.19
3441	CB	LEU	B	1119	8.465	51.252	46.982	1	57.62
3442	CG	LEU	B	1119	9.475	52.395	47.071	1	57.94
3443	CD1	LEU	B	1119	9.294	53.145	48.369	1	61.13
3444	CD2	LEU	B	1119	10.889	51.844	46.977	1	57.55
3445	N	MET	B	1120	6.07	52.258	45.1	1	59.1
3446	CA	MET	B	1120	5.588	53.199	44.086	1	62.27
3447	C	MET	B	1120	4.165	53.716	44.29	1	65.88
3448	O	MET	B	1120	3.782	54.753	43.749	1	64.99
3449	CB	MET	B	1120	5.661	52.564	42.697	1	59.98
3450	CG	MET	B	1120	7.043	52.365	42.158	1	54.51
3451	SD	MET	B	1120	6.871	51.966	40.439	1	55.01
3452	CE	MET	B	1120	7.327	50.238	40.4	1	48.49
3453	N	LYS	B	1121	3.364	52.929	44.995	1	70.84
3454	CA	LYS	B	1121	1.981	53.263	45.286	1	72.19
3455	C	LYS	B	1121	1.924	54.382	46.327	1	75.33
3456	O	LYS	B	1121	1.054	55.244	46.266	1	75.8
3457	CB	LYS	B	1121	1.291	52.01	45.815	1	70.77
3458	CG	LYS	B	1121	-0.195	52.104	45.963	1	74.66
3459	CD	LYS	B	1121	-0.739	50.731	46.312	1	80.54
3460	CE	LYS	B	1121	-2.258	50.681	46.314	1	81.02
3461	NZ	LYS	B	1121	-2.715	49.283	46.558	1	82.34
3462	N	HIS	B	1122	2.877	54.371	47.259	1	79.37
3463	CA	HIS	B	1122	2.941	55.355	48.339	1	84.05
3464	C	HIS	B	1122	3.634	56.648	47.932	1	83.81
3465	O	HIS	B	1122	3.183	57.738	48.287	1	83.68
3466	CB	HIS	B	1122	3.655	54.762	49.577	1	89.84
3467	CG	HIS	B	1122	2.937	53.6	50.214	1	97.14
3468	ND1	HIS	B	1122	1.748	53.09	49.73	1	98.38
3469	CD2	HIS	B	1122	3.253	52.846	51.297	1	98.8
3470	CE1	HIS	B	1122	1.363	52.074	50.484	1	99.03
3471	NE2	HIS	B	1122	2.26	51.904	51.443	1	100
3472	N	GLU	B	1123	4.705	56.53	47.153	1	83.96

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3473	CA	GLU	B	1123	5.467	57.705	46.743	1	83.63
3474	C	GLU	B	1123	5.969	57.726	45.295	1	82.16
3475	O	GLU	B	1123	6.013	56.695	44.619	1	80.04
3476	CB	GLU	B	1123	6.647	57.901	47.71	1	84.93
3477	CG	GLU	B	1123	7.53	56.669	47.86	1	85.12
3478	CD	GLU	B	1123	8.589	56.83	48.925	1	86.79
3479	OE1	GLU	B	1123	8.277	56.587	50.115	1	86.76
3480	OE2	GLU	B	1123	9.732	57.189	48.566	1	86.46
3481	N	LYS	B	1124	6.28	58.933	44.814	1	82.56
3482	CA	LYS	B	1124	6.821	59.132	43.465	1	81.06
3483	C	LYS	B	1124	8.317	59.052	43.668	1	77.78
3484	O	LYS	B	1124	8.841	59.618	44.636	1	78.5
3485	CB	LYS	B	1124	6.458	60.504	42.892	1	84.26
3486	CG	LYS	B	1124	6.548	60.575	41.366	1	86.98
3487	CD	LYS	B	1124	5.693	59.475	40.717	1	91.96
3488	CE	LYS	B	1124	5.502	59.697	39.216	1	94.56
3489	NZ	LYS	B	1124	4.471	60.739	38.898	1	96.11
3490	N	LEU	B	1125	9.003	58.395	42.741	1	71.62
3491	CA	LEU	B	1125	10.426	58.19	42.889	1	67.92
3492	C	LEU	B	1125	11.399	59.349	42.723	1	68.88
3493	O	LEU	B	1125	11.86	59.913	43.716	1	71.34
3494	CB	LEU	B	1125	10.845	56.958	42.1	1	64.73
3495	CG	LEU	B	1125	10.259	55.671	42.703	1	59.06
3496	CD1	LEU	B	1125	10.574	54.504	41.839	1	54.98
3497	CD2	LEU	B	1125	10.797	55.439	44.109	1	54.83
3498	N	GLY	B	1126	11.736	59.716	41.501	1	67.61
3499	CA	GLY	B	1126	12.683	60.804	41.356	1	70.66
3500	C	GLY	B	1126	13.93	60.337	40.63	1	73.02
3501	O	GLY	B	1126	14.472	59.271	40.922	1	72.39
3502	N	GLU	B	1127	14.401	61.173	39.711	1	74.64
3503	CA	GLU	B	1127	15.554	60.88	38.874	1	76.17
3504	C	GLU	B	1127	16.695	60.069	39.461	1	74.33
3505	O	GLU	B	1127	17.004	58.999	38.945	1	72.9
3506	CB	GLU	B	1127	16.087	62.162	38.234	1	81.52
3507	CG	GLU	B	1127	15.108	62.779	37.241	1	86.13
3508	CD	GLU	B	1127	15.767	63.745	36.27	1	89.36
3509	OE1	GLU	B	1127	16.875	63.441	35.766	1	89.13
3510	OE2	GLU	B	1127	15.158	64.804	35.998	1	92.24
3511	N	ASP	B	1128	17.328	60.567	40.519	1	73.57
3512	CA	ASP	B	1128	18.445	59.84	41.116	1	73.67
3513	C	ASP	B	1128	18.035	58.45	41.601	1	72.87
3514	O	ASP	B	1128	18.734	57.467	41.336	1	73.04
3515	CB	ASP	B	1128	19.077	60.646	42.258	1	75.81
3516	CG	ASP	B	1128	20.069	61.706	41.765	1	77.88
3517	OD1	ASP	B	1128	20.028	62.093	40.572	1	76.08
3518	OD2	ASP	B	1128	20.902	62.154	42.586	1	78.33
3519	N	ARG	B	1129	16.881	58.373	42.269	1	71.72
3520	CA	ARG	B	1129	16.342	57.116	42.809	1	69.85
3521	C	ARG	B	1129	16.04	56.084	41.718	1	65.08
3522	O	ARG	B	1129	16.503	54.943	41.771	1	60.98
3523	CB	ARG	B	1129	15.058	57.391	43.596	1	74.44
3524	CG	ARG	B	1129	15.165	57.417	45.108	1	79.34
3525	CD	ARG	B	1129	13.729	57.482	45.602	1	86.88
3526	NE	ARG	B	1129	13.599	57.222	46.985	1	95.02
3527	CZ	ARG	B	1129	13.062	56.309	47.786	1	98.4
3528	NH1	ARG	B	1129	12.4	55.196	47.479	1	98.08

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3529	NH2	ARG	B	1129	13.275	56.613	49.054	1	100
3530	N	ILE	B	1130	15.239	56.501	40.744	1	61.08
3531	CA	ILE	B	1130	14.856	55.648	39.632	1	56.02
3532	C	ILE	B	1130	16.072	55.059	38.945	1	55.95
3533	O	ILE	B	1130	16.047	53.896	38.555	1	57.22
3534	CB	ILE	B	1130	14.014	56.434	38.618	1	53.66
3535	CG1	ILE	B	1130	12.74	56.926	39.3	1	54.96
3536	CG2	ILE	B	1130	13.699	55.578	37.408	1	53.66
3537	CD1	ILE	B	1130	11.897	57.876	38.479	1	55.23
3538	N	GLN	B	1131	17.137	55.856	38.821	1	57.03
3539	CA	GLN	B	1131	18.384	55.423	38.182	1	57.03
3540	C	GLN	B	1131	19.067	54.345	38.994	1	56.82
3541	O	GLN	B	1131	19.425	53.283	38.48	1	57.84
3542	CB	GLN	B	1131	19.371	56.58	38.027	1	59.35
3543	CG	GLN	B	1131	20.68	56.139	37.365	1	63.44
3544	CD	GLN	B	1131	21.801	57.156	37.493	1	64.89
3545	OE1	GLN	B	1131	22.522	57.429	36.53	1	64.54
3546	NE2	GLN	B	1131	21.976	57.694	38.694	1	68.97
3547	N	PHE	B	1132	19.268	54.64	40.269	1	55.63
3548	CA	PHE	B	1132	19.913	53.7	41.168	1	52.85
3549	C	PHE	B	1132	19.169	52.372	41.178	1	49.79
3550	O	PHE	B	1132	19.774	51.307	41.038	1	51.14
3551	CB	PHE	B	1132	19.95	54.278	42.587	1	53.09
3552	CG	PHE	B	1132	20.853	53.528	43.521	1	53.2
3553	CD1	PHE	B	1132	22.053	52.968	43.06	1	54.16
3554	CD2	PHE	B	1132	20.514	53.384	44.854	1	50.23
3555	CE1	PHE	B	1132	22.9	52.273	43.918	1	53.87
3556	CE2	PHE	B	1132	21.354	52.691	45.723	1	55.54
3557	CZ	PHE	B	1132	22.553	52.132	45.251	1	54.71
3558	N	LEU	B	1133	17.851	52.445	41.305	1	44.05
3559	CA	LEU	B	1133	17.052	51.238	41.358	1	41.13
3560	C	LEU	B	1133	17.215	50.404	40.118	1	42.01
3561	O	LEU	B	1133	17.571	49.24	40.218	1	42.85
3562	CB	LEU	B	1133	15.578	51.553	41.62	1	35.84
3563	CG	LEU	B	1133	15.285	52.134	43.011	1	32.28
3564	CD1	LEU	B	1133	13.802	52.374	43.2	1	35.05
3565	CD2	LEU	B	1133	15.803	51.202	44.074	1	32.13
3566	N	VAL	B	1134	17.079	51.032	38.95	1	43.76
3567	CA	VAL	B	1134	17.178	50.314	37.671	1	41.86
3568	C	VAL	B	1134	18.558	49.742	37.409	1	45.23
3569	O	VAL	B	1134	18.697	48.68	36.792	1	49.26
3570	CB	VAL	B	1134	16.751	51.193	36.484	1	36.34
3571	CG1	VAL	B	1134	16.726	50.378	35.205	1	31.6
3572	CG2	VAL	B	1134	15.381	51.776	36.738	1	37.61
3573	N	TYR	B	1135	19.576	50.453	37.877	1	47.4
3574	CA	TYR	B	1135	20.954	50.017	37.718	1	48.59
3575	C	TYR	B	1135	21.077	48.657	38.404	1	49.03
3576	O	TYR	B	1135	21.611	47.705	37.834	1	47.74
3577	CB	TYR	B	1135	21.895	51.026	38.388	1	52.16
3578	CG	TYR	B	1135	23.359	50.648	38.29	1	57.47
3579	CD1	TYR	B	1135	23.928	50.297	37.058	1	58.3
3580	CD2	TYR	B	1135	24.171	50.619	39.424	1	58.11
3581	CE1	TYR	B	1135	25.266	49.93	36.959	1	58.53
3582	CE2	TYR	B	1135	25.513	50.246	39.334	1	60.23
3583	CZ	TYR	B	1135	26.053	49.905	38.097	1	61.07
3584	OH	TYR	B	1135	27.382	49.535	37.994	1	66.1

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3585	N	GLN	B	1136	20.525	48.583	39.615	1	48.47
3586	CA	GLN	B	1136	20.533	47.374	40.419	1	47.8
3587	C	GLN	B	1136	19.713	46.227	39.804	1	48.71
3588	O	GLN	B	1136	20.118	45.062	39.878	1	49.82
3589	CB	GLN	B	1136	20.044	47.691	41.816	1	50.54
3590	CG	GLN	B	1136	20.795	48.813	42.479	1	48.71
3591	CD	GLN	B	1136	20.47	48.908	43.943	1	51.78
3592	OE1	GLN	B	1136	20.809	48.009	44.724	1	53.24
3593	NE2	GLN	B	1136	19.804	49.99	44.334	1	48.84
3594	N	MET	B	1137	18.562	46.536	39.215	1	44.32
3595	CA	MET	B	1137	17.775	45.493	38.564	1	46.03
3596	C	MET	B	1137	18.674	44.815	37.53	1	49.34
3597	O	MET	B	1137	18.766	43.58	37.457	1	50.26
3598	CB	MET	B	1137	16.598	46.098	37.805	1	40.63
3599	CG	MET	B	1137	15.353	46.242	38.588	1	42.48
3600	SD	MET	B	1137	14.318	47.431	37.791	1	47.34
3601	CE	MET	B	1137	14.255	48.7	39.048	1	42.91
3602	N	LEU	B	1138	19.366	45.661	36.766	1	48.43
3603	CA	LEU	B	1138	20.234	45.229	35.695	1	45.62
3604	C	LEU	B	1138	21.501	44.467	36.066	1	45.99
3605	O	LEU	B	1138	21.898	43.554	35.339	1	44.39
3606	CB	LEU	B	1138	20.506	46.415	34.78	1	43.96
3607	CG	LEU	B	1138	19.232	46.802	34.017	1	41.59
3608	CD1	LEU	B	1138	19.445	48.074	33.245	1	42.5
3609	CD2	LEU	B	1138	18.843	45.669	33.069	1	38.1
3610	N	LYS	B	1139	22.14	44.816	37.179	1	46.62
3611	CA	LYS	B	1139	23.337	44.071	37.576	1	46.94
3612	C	LYS	B	1139	22.842	42.694	38.006	1	45.46
3613	O	LYS	B	1139	23.434	41.667	37.688	1	47.02
3614	CB	LYS	B	1139	24.088	44.755	38.728	1	48.43
3615	CG	LYS	B	1139	24.737	46.083	38.351	1	54.08
3616	CD	LYS	B	1139	26.007	46.372	39.143	1	58.36
3617	CE	LYS	B	1139	25.758	46.451	40.654	1	66.2
3618	NZ	LYS	B	1139	27.03	46.525	41.469	1	67.31
3619	N	GLY	B	1140	21.703	42.688	38.682	1	42.91
3620	CA	GLY	B	1140	21.136	41.445	39.131	1	38.97
3621	C	GLY	B	1140	20.835	40.616	37.923	1	41.74
3622	O	GLY	B	1140	21.195	39.435	37.861	1	42.79
3623	N	LEU	B	1141	20.247	41.265	36.92	1	43.16
3624	CA	LEU	B	1141	19.887	40.577	35.692	1	44.48
3625	C	LEU	B	1141	21.094	40.037	34.951	1	47.53
3626	O	LEU	B	1141	21.101	38.867	34.557	1	49.29
3627	CB	LEU	B	1141	19.096	41.483	34.781	1	40.49
3628	CG	LEU	B	1141	17.649	41.057	34.565	1	40.66
3629	CD1	LEU	B	1141	17.207	41.641	33.228	1	42.75
3630	CD2	LEU	B	1141	17.518	39.547	34.53	1	35.6
3631	N	ARG	B	1142	22.12	40.877	34.799	1	49.33
3632	CA	ARG	B	1142	23.34	40.474	34.107	1	52.44
3633	C	ARG	B	1142	23.904	39.219	34.753	1	54.8
3634	O	ARG	B	1142	24.424	38.343	34.051	1	55.56
3635	CB	ARG	B	1142	24.398	41.574	34.125	1	53.1
3636	CG	ARG	B	1142	25.461	41.382	33.054	1	55.22
3637	CD	ARG	B	1142	26.847	41.755	33.538	1	61.94
3638	NE	ARG	B	1142	26.895	43.071	34.173	1	68.45
3639	CZ	ARG	B	1142	27.861	43.467	34.998	1	71.59
3640	NH1	ARG	B	1142	28.863	42.648	35.282	1	76.4

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3641	NH2	ARG	B	1142	27.806	44.661	35.577	1	73.39
3642	N	TYR	B	1143	23.795	39.139	36.083	1	54.15
3643	CA	TYR	B	1143	24.267	37.976	36.802	1	54.04
3644	C	TYR	B	1143	23.401	36.768	36.452	1	55
3645	O	TYR	B	1143	23.902	35.763	35.948	1	56.08
3646	CB	TYR	B	1143	24.24	38.206	38.312	1	55.69
3647	CG	TYR	B	1143	24.59	36.957	39.109	1	54.84
3648	CD1	TYR	B	1143	25.91	36.512	39.197	1	54.34
3649	CD2	TYR	B	1143	23.595	36.177	39.697	1	52.78
3650	CE1	TYR	B	1143	26.231	35.319	39.839	1	51.48
3651	CE2	TYR	B	1143	23.9	34.986	40.334	1	53.29
3652	CZ	TYR	B	1143	25.224	34.56	40.402	1	53.23
3653	OH	TYR	B	1143	25.54	33.374	41.029	1	52.52
3654	N	ILE	B	1144	22.1	36.875	36.704	1	53.33
3655	CA	ILE	B	1144	21.177	35.778	36.426	1	50.27
3656	C	ILE	B	1144	21.347	35.226	35.011	1	53.25
3657	O	ILE	B	1144	21.354	34.014	34.806	1	56.43
3658	CB	ILE	B	1144	19.732	36.242	36.637	1	46.32
3659	CG1	ILE	B	1144	19.554	36.678	38.083	1	40.16
3660	CG2	ILE	B	1144	18.745	35.118	36.34	1	44.48
3661	CD1	ILE	B	1144	18.392	37.594	38.271	1	41.57
3662	N	HIS	B	1145	21.538	36.123	34.049	1	53.89
3663	CA	HIS	B	1145	21.71	35.745	32.651	1	53.63
3664	C	HIS	B	1145	23.061	35.143	32.313	1	55.06
3665	O	HIS	B	1145	23.132	34.137	31.603	1	55.93
3666	CB	HIS	B	1145	21.446	36.945	31.755	1	53.17
3667	CG	HIS	B	1145	20.003	37.313	31.673	1	51.03
3668	ND1	HIS	B	1145	19.575	38.535	31.207	1	49.45
3669	CD2	HIS	B	1145	18.89	36.609	31.979	1	49.05
3670	CE1	HIS	B	1145	18.255	38.567	31.227	1	51.87
3671	NE2	HIS	B	1145	17.815	37.409	31.69	1	51.75
3672	N	ALA	B	1146	24.133	35.785	32.773	1	56.94
3673	CA	ALA	B	1146	25.491	35.271	32.539	1	57.72
3674	C	ALA	B	1146	25.566	33.856	33.098	1	55.26
3675	O	ALA	B	1146	26.329	33.015	32.617	1	57.5
3676	CB	ALA	B	1146	26.537	36.16	33.226	1	56.09
3677	N	ALA	B	1147	24.743	33.606	34.11	1	52.41
3678	CA	ALA	B	1147	24.676	32.31	34.742	1	52.4
3679	C	ALA	B	1147	23.785	31.378	33.932	1	53.33
3680	O	ALA	B	1147	23.518	30.25	34.356	1	56.66
3681	CB	ALA	B	1147	24.156	32.451	36.156	1	47
3682	N	GLY	B	1148	23.331	31.853	32.771	1	53.31
3683	CA	GLY	B	1148	22.464	31.058	31.904	1	53.81
3684	C	GLY	B	1148	21.023	30.837	32.372	1	51.69
3685	O	GLY	B	1148	20.321	29.973	31.842	1	50.84
3686	N	ILE	B	1149	20.602	31.6	33.38	1	50.99
3687	CA	ILE	B	1149	19.249	31.531	33.941	1	49.74
3688	C	ILE	B	1149	18.325	32.594	33.301	1	48.79
3689	O	ILE	B	1149	18.779	33.633	32.802	1	44.6
3690	CB	ILE	B	1149	19.281	31.772	35.488	1	48.77
3691	CG1	ILE	B	1149	20.061	30.663	36.184	1	50.52
3692	CG2	ILE	B	1149	17.888	31.843	36.069	1	47.26
3693	CD1	ILE	B	1149	20.388	30.955	37.632	1	50.13
3694	N	ILE	B	1150	17.031	32.291	33.28	1	47.03
3695	CA	ILE	B	1150	16.029	33.208	32.764	1	45.69
3696	C	ILE	B	1150	15.001	33.335	33.896	1	47.53

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3697	O	ILE	B	1150	14.569	32.326	34.478	1	47.87
3698	CB	ILE	B	1150	15.402	32.702	31.45	1	45.45
3699	CG1	ILE	B	1150	14.366	33.696	30.957	1	42.45
3700	CG2	ILE	B	1150	14.792	31.315	31.624	1	46.3
3701	CD1	ILE	B	1150	14.018	33.491	29.527	1	43.98
3702	N	HIS	B	1151	14.635	34.575	34.223	1	44.2
3703	CA	HIS	B	1151	13.73	34.841	35.321	1	37.69
3704	C	HIS	B	1151	12.252	34.662	35.031	1	41.01
3705	O	HIS	B	1151	11.512	34.109	35.861	1	40.05
3706	CB	HIS	B	1151	13.994	36.241	35.882	1	37.84
3707	CG	HIS	B	1151	13.195	36.547	37.104	1	30.23
3708	ND1	HIS	B	1151	11.845	36.824	37.052	1	30.05
3709	CD2	HIS	B	1151	13.523	36.513	38.416	1	31.02
3710	CE1	HIS	B	1151	11.376	36.933	38.285	1	32.07
3711	NE2	HIS	B	1151	12.375	36.749	39.132	1	26.47
3712	N	ARG	B	1152	11.807	35.217	33.906	1	41.8
3713	CA	ARG	B	1152	10.407	35.129	33.465	1	42.27
3714	C	ARG	B	1152	9.3	35.758	34.32	1	41.18
3715	O	ARG	B	1152	8.134	35.367	34.192	1	43.19
3716	CB	ARG	B	1152	10.043	33.68	33.16	1	39.46
3717	CG	ARG	B	1152	10.84	33.125	32.027	1	41.9
3718	CD	ARG	B	1152	11.24	31.746	32.375	1	42.14
3719	NE	ARG	B	1152	10.593	30.76	31.527	1	47.05
3720	CZ	ARG	B	1152	10.056	29.636	31.976	1	43.86
3721	NH1	ARG	B	1152	10.068	29.377	33.265	1	41.3
3722	NH2	ARG	B	1152	9.627	28.716	31.125	1	46.12
3723	N	ASP	B	1153	9.64	36.691	35.203	1	34.87
3724	CA	ASP	B	1153	8.597	37.328	35.988	1	33.15
3725	C	ASP	B	1153	8.991	38.637	36.669	1	34.98
3726	O	ASP	B	1153	8.511	38.949	37.755	1	32.43
3727	CB	ASP	B	1153	8.034	36.368	37.019	1	31.59
3728	CG	ASP	B	1153	6.608	36.738	37.428	1	38.53
3729	OD1	ASP	B	1153	5.83	37.15	36.54	1	40.91
3730	OD2	ASP	B	1153	6.25	36.64	38.623	1	36.3
3731	N	LEU	B	1154	9.864	39.411	36.039	1	31.7
3732	CA	LEU	B	1154	10.268	40.657	36.643	1	33.64
3733	C	LEU	B	1154	9.09	41.626	36.595	1	31.96
3734	O	LEU	B	1154	8.514	41.89	35.554	1	32.06
3735	CB	LEU	B	1154	11.492	41.228	35.924	1	33.58
3736	CG	LEU	B	1154	12.621	40.214	36.031	1	36.54
3737	CD1	LEU	B	1154	13.852	40.778	35.404	1	39.3
3738	CD2	LEU	B	1154	12.876	39.873	37.506	1	33.9
3739	N	LYS	B	1155	8.673	42.074	37.757	1	31.22
3740	CA	LYS	B	1155	7.578	43.005	37.854	1	33.96
3741	C	LYS	B	1155	7.878	43.708	39.137	1	35.23
3742	O	LYS	B	1155	8.661	43.209	39.931	1	36.46
3743	CB	LYS	B	1155	6.236	42.285	37.907	1	35.04
3744	CG	LYS	B	1155	6.012	41.375	39.086	1	36.77
3745	CD	LYS	B	1155	4.832	40.474	38.802	1	40.8
3746	CE	LYS	B	1155	4.382	39.777	40.057	1	43.85
3747	NZ	LYS	B	1155	2.96	39.391	39.94	1	46.98
3748	N	PRO	B	1156	7.276	44.88	39.361	1	36.93
3749	CA	PRO	B	1156	7.527	45.632	40.592	1	37.08
3750	C	PRO	B	1156	7.374	44.792	41.865	1	39.23
3751	O	PRO	B	1156	8.157	44.92	42.805	1	43.87
3752	CB	PRO	B	1156	6.47	46.734	40.523	1	41.2

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3753	CG	PRO	B	1156	6.275	46.932	39.024	1	37.21
3754	CD	PRO	B	1156	6.21	45.512	38.555	1	36.35
3755	N	GLY	B	1157	6.376	43.914	41.878	1	38.41
3756	CA	GLY	B	1157	6.141	43.076	43.037	1	37.48
3757	C	GLY	B	1157	7.209	42.039	43.348	1	36.76
3758	O	GLY	B	1157	7.212	41.466	44.433	1	39.68
3759	N	ASN	B	1158	8.069	41.744	42.391	1	33.82
3760	CA	ASN	B	1158	9.139	40.788	42.613	1	37.83
3761	C	ASN	B	1158	10.473	41.493	42.694	1	38.7
3762	O	ASN	B	1158	11.476	40.95	42.248	1	38.46
3763	CB	ASN	B	1158	9.222	39.743	41.505	1	38.35
3764	CG	ASN	B	1158	7.994	38.896	41.417	1	40.45
3765	OD1	ASN	B	1158	7.414	38.505	42.436	1	35.16
3766	ND2	ASN	B	1158	7.573	38.606	40.19	1	38.65
3767	N	LEU	B	1159	10.473	42.725	43.196	1	38.47
3768	CA	LEU	B	1159	11.714	43.473	43.359	1	39.51
3769	C	LEU	B	1159	11.681	44.133	44.723	1	40.21
3770	O	LEU	B	1159	10.867	45.03	44.946	1	43.09
3771	CB	LEU	B	1159	11.869	44.542	42.28	1	37.49
3772	CG	LEU	B	1159	11.956	44.088	40.824	1	38.03
3773	CD1	LEU	B	1159	11.944	45.331	39.963	1	29.48
3774	CD2	LEU	B	1159	13.208	43.208	40.554	1	36.35
3775	N	ALA	B	1160	12.559	43.692	45.628	1	38.14
3776	CA	ALA	B	1160	12.608	44.242	46.983	1	41.34
3777	C	ALA	B	1160	13.56	45.428	47.111	1	41.67
3778	O	ALA	B	1160	14.634	45.45	46.521	1	45.76
3779	CB	ALA	B	1160	12.954	43.161	47.974	1	39.03
3780	N	VAL	B	1161	13.167	46.397	47.916	1	41.49
3781	CA	VAL	B	1161	13.954	47.606	48.1	1	45.96
3782	C	VAL	B	1161	13.927	47.998	49.568	1	46.67
3783	O	VAL	B	1161	12.847	48.223	50.116	1	47.58
3784	CB	VAL	B	1161	13.309	48.779	47.309	1	46.19
3785	CG1	VAL	B	1161	14.121	50.031	47.469	1	49.32
3786	CG2	VAL	B	1161	13.165	48.427	45.85	1	44.43
3787	N	ASN	B	1162	15.092	48.109	50.205	1	47.85
3788	CA	ASN	B	1162	15.123	48.506	51.615	1	50.5
3789	C	ASN	B	1162	15.252	50.021	51.847	1	53.04
3790	O	ASN	B	1162	15.29	50.8	50.893	1	51.83
3791	CB	ASN	B	1162	16.217	47.751	52.369	1	50.67
3792	CG	ASN	B	1162	17.599	48.075	51.87	1	54
3793	OD1	ASN	B	1162	17.852	49.168	51.346	1	49.99
3794	ND2	ASN	B	1162	18.519	47.113	52.023	1	54.01
3795	N	GLU	B	1163	15.332	50.423	53.116	1	56.87
3796	CA	GLU	B	1163	15.444	51.834	53.512	1	61.04
3797	C	GLU	B	1163	16.598	52.572	52.847	1	61.38
3798	O	GLU	B	1163	16.512	53.781	52.623	1	62.21
3799	CB	GLU	B	1163	15.631	51.968	55.024	1	66.73
3800	CG	GLU	B	1163	14.589	51.295	55.909	1	74.14
3801	CD	GLU	B	1163	14.869	51.531	57.391	1	78.04
3802	OE1	GLU	B	1163	16.024	51.294	57.844	1	80.69
3803	OE2	GLU	B	1163	13.935	51.973	58.097	1	79.71
3804	N	ASP	B	1164	17.695	51.859	52.604	1	60.92
3805	CA	ASP	B	1164	18.875	52.439	51.97	1	62.75
3806	C	ASP	B	1164	18.841	52.303	50.44	1	62.79
3807	O	ASP	B	1164	19.881	52.346	49.77	1	64.03
3808	CB	ASP	B	1164	20.148	51.799	52.541	1	64.9

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3809	CG	ASP	B	1164	20.409	52.198	53.99	1	70.14
3810	OD1	ASP	B	1164	19.718	53.106	54.513	1	72.87
3811	OD2	ASP	B	1164	21.319	51.608	54.612	1	73.36
3812	N	CYS	B	1165	17.634	52.157	49.903	1	61.53
3813	CA	CYS	B	1165	17.4	52.004	48.47	1	60.6
3814	C	CYS	B	1165	18.173	50.895	47.763	1	55.92
3815	O	CYS	B	1165	18.451	50.986	46.57	1	55.05
3816	CB	CYS	B	1165	17.549	53.344	47.739	1	64.16
3817	SG	CYS	B	1165	15.997	54.299	47.695	1	75.2
3818	N	GLU	B	1166	18.491	49.835	48.497	1	52.23
3819	CA	GLU	B	1166	19.191	48.696	47.918	1	51.52
3820	C	GLU	B	1166	18.129	47.746	47.377	1	49.56
3821	O	GLU	B	1166	17.038	47.62	47.951	1	52.89
3822	CB	GLU	B	1166	20.076	48.033	48.971	1	56.91
3823	CG	GLU	B	1166	21.022	49.044	49.621	1	61.48
3824	CD	GLU	B	1166	21.976	48.429	50.62	1	65.34
3825	OE1	GLU	B	1166	21.493	47.855	51.615	1	68.02
3826	OE2	GLU	B	1166	23.208	48.545	50.425	1	63.05
3827	N	LEU	B	1167	18.41	47.123	46.242	1	43.77
3828	CA	LEU	B	1167	17.435	46.245	45.642	1	38.48
3829	C	LEU	B	1167	17.915	44.82	45.491	1	40.25
3830	O	LEU	B	1167	19.106	44.574	45.306	1	40.47
3831	CB	LEU	B	1167	17.019	46.808	44.276	1	39.35
3832	CG	LEU	B	1167	16.113	46.007	43.309	1	38.05
3833	CD1	LEU	B	1167	15.269	46.928	42.471	1	32.6
3834	CD2	LEU	B	1167	16.921	45.079	42.409	1	38.83
3835	N	LYS	B	1168	16.968	43.89	45.575	1	39.06
3836	CA	LYS	B	1168	17.233	42.461	45.383	1	42.57
3837	C	LYS	B	1168	16.053	41.856	44.592	1	40.77
3838	O	LYS	B	1168	14.887	42.08	44.899	1	41.04
3839	CB	LYS	B	1168	17.451	41.733	46.724	1	45.45
3840	CG	LYS	B	1168	18.852	41.937	47.345	1	47.6
3841	CD	LYS	B	1168	18.883	41.639	48.845	1	51.98
3842	CE	LYS	B	1168	20.306	41.553	49.405	1	57.36
3843	NZ	LYS	B	1168	20.995	40.257	49.063	1	60.39
3844	N	ILE	B	1169	16.37	41.193	43.494	1	38.08
3845	CA	ILE	B	1169	15.364	40.565	42.659	1	39.04
3846	C	ILE	B	1169	14.774	39.378	43.4	1	41.65
3847	O	ILE	B	1169	15.509	38.53	43.925	1	42.84
3848	CB	ILE	B	1169	15.983	40.093	41.344	1	39.72
3849	CG1	ILE	B	1169	16.444	41.311	40.547	1	34.39
3850	CG2	ILE	B	1169	15.01	39.204	40.567	1	39.03
3851	CD1	ILE	B	1169	17.087	40.976	39.258	1	34.86
3852	N	LEU	B	1170	13.448	39.349	43.482	1	38.67
3853	CA	LEU	B	1170	12.75	38.278	44.165	1	39.63
3854	C	LEU	B	1170	12.047	37.313	43.234	1	39.3
3855	O	LEU	B	1170	12.133	37.402	42.02	1	41.56
3856	CB	LEU	B	1170	11.688	38.868	45.087	1	36.72
3857	CG	LEU	B	1170	12.138	39.823	46.176	1	36.16
3858	CD1	LEU	B	1170	10.912	40.462	46.8	1	30.53
3859	CD2	LEU	B	1170	12.998	39.088	47.217	1	36.94
3860	N	ASP	B	1171	11.368	36.357	43.851	1	44.43
3861	CA	ASP	B	1171	10.535	35.378	43.162	1	41.68
3862	C	ASP	B	1171	11.11	34.617	42.001	1	41.67
3863	O	ASP	B	1171	10.858	34.961	40.852	1	43.91
3864	CB	ASP	B	1171	9.255	36.071	42.69	1	42.47

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3865	CG	ASP	B	1171	8.075	35.127	42.578	1	45.71
3866	OD1	ASP	B	1171	8.295	33.891	42.466	1	45.02
3867	OD2	ASP	B	1171	6.923	35.631	42.62	1	36.4
3868	N	PHE	B	1172	11.857	33.56	42.274	1	43.92
3869	CA	PHE	B	1172	12.361	32.758	41.174	1	42.77
3870	C	PHE	B	1172	11.424	31.6	40.909	1	43.77
3871	O	PHE	B	1172	11.796	30.635	40.264	1	50.44
3872	CB	PHE	B	1172	13.77	32.292	41.445	1	39.54
3873	CG	PHE	B	1172	14.785	33.339	41.165	1	41.01
3874	CD1	PHE	B	1172	14.953	34.404	42.037	1	39.05
3875	CD2	PHE	B	1172	15.538	33.301	39.994	1	42.1
3876	CE1	PHE	B	1172	15.86	35.426	41.745	1	40.54
3877	CE2	PHE	B	1172	16.448	34.315	39.692	1	39.85
3878	CZ	PHE	B	1172	16.606	35.377	40.571	1	40.67
3879	N	GLY	B	1173	10.174	31.756	41.341	1	44.58
3880	CA	GLY	B	1173	9.154	30.73	41.17	1	47.24
3881	C	GLY	B	1173	8.817	30.344	39.744	1	48.98
3882	O	GLY	B	1173	8.271	29.268	39.509	1	50.09
3883	N	LEU	B	1174	9.113	31.23	38.796	1	47.5
3884	CA	LEU	B	1174	8.86	30.958	37.396	1	44.45
3885	C	LEU	B	1174	10.175	30.92	36.64	1	44.98
3886	O	LEU	B	1174	10.18	30.786	35.425	1	49.18
3887	CB	LEU	B	1174	7.959	32.025	36.795	1	46.57
3888	CG	LEU	B	1174	7.335	31.658	35.449	1	49.49
3889	CD1	LEU	B	1174	6.384	30.477	35.635	1	52.43
3890	CD2	LEU	B	1174	6.585	32.852	34.878	1	54.72
3891	N	ALA	B	1175	11.295	31.019	37.348	1	43.44
3892	CA	ALA	B	1175	12.597	30.992	36.694	1	42.54
3893	C	ALA	B	1175	13.053	29.576	36.298	1	43.79
3894	O	ALA	B	1175	12.481	28.576	36.74	1	38.37
3895	CB	ALA	B	1175	13.614	31.648	37.571	1	40.52
3896	N	ARG	B	1176	14.066	29.511	35.432	1	47.34
3897	CA	ARG	B	1176	14.631	28.248	34.956	1	50.47
3898	C	ARG	B	1176	15.938	28.524	34.223	1	53.83
3899	O	ARG	B	1176	16.373	29.68	34.108	1	52.97
3900	CB	ARG	B	1176	13.667	27.551	33.992	1	54.56
3901	CG	ARG	B	1176	13.876	27.945	32.523	1	57.15
3902	CD	ARG	B	1176	12.712	27.603	31.618	1	59.93
3903	NE	ARG	B	1176	12.533	26.177	31.324	1	63.13
3904	CZ	ARG	B	1176	13.4	25.413	30.662	1	61.48
3905	NH1	ARG	B	1176	14.547	25.912	30.236	1	63.98
3906	NH2	ARG	B	1176	13.06	24.185	30.3	1	58.38
3907	N	GLN	B	1177	16.567	27.451	33.745	1	57.87
3908	CA	GLN	B	1177	17.808	27.555	32.985	1	62.7
3909	C	GLN	B	1177	17.404	27.809	31.532	1	63.38
3910	O	GLN	B	1177	16.599	27.068	30.969	1	62.96
3911	CB	GLN	B	1177	18.593	26.249	33.08	1	67.17
3912	CG	GLN	B	1177	19.975	26.305	32.45	1	74.7
3913	CD	GLN	B	1177	20.57	24.92	32.26	1	80.17
3914	OE1	GLN	B	1177	19.995	24.077	31.559	1	83.06
3915	NE2	GLN	B	1177	21.716	24.67	32.889	1	80.44
3916	N	ALA	B	1178	17.94	28.866	30.934	1	63.49
3917	CA	ALA	B	1178	17.599	29.202	29.562	1	64.11
3918	C	ALA	B	1178	17.903	28.05	28.622	1	65.94
3919	O	ALA	B	1178	18.943	27.397	28.742	1	69.41
3920	CB	ALA	B	1178	18.339	30.459	29.127	1	59.96

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3921	N	ASP	B	1179	16.964	27.773	27.724	1	68.01
3922	CA	ASP	B	1179	17.115	26.712	26.736	1	69.02
3923	C	ASP	B	1179	16.449	27.178	25.445	1	69.54
3924	O	ASP	B	1179	16.035	28.333	25.341	1	69.63
3925	CB	ASP	B	1179	16.483	25.418	27.246	1	69.96
3926	CG	ASP	B	1179	16.933	24.192	26.46	1	74.7
3927	OD1	ASP	B	1179	18.092	24.163	25.974	1	75.27
3928	OD2	ASP	B	1179	16.118	23.252	26.33	1	75.59
3929	N	SER	B	1180	16.357	26.298	24.456	1	70.8
3930	CA	SER	B	1180	15.753	26.656	23.175	1	69.23
3931	C	SER	B	1180	14.234	26.679	23.136	1	68.81
3932	O	SER	B	1180	13.647	27.604	22.579	1	69.52
3933	CB	SER	B	1180	16.294	25.759	22.064	1	69.96
3934	OG	SER	B	1180	17.59	26.187	21.685	1	71.51
3935	N	GLU	B	1181	13.599	25.675	23.73	1	69.72
3936	CA	GLU	B	1181	12.144	25.597	23.726	1	71.3
3937	C	GLU	B	1181	11.594	25.559	25.15	1	70.66
3938	O	GLU	B	1181	11.546	24.498	25.777	1	73.66
3939	CB	GLU	B	1181	11.698	24.353	22.958	1	74.63
3940	CG	GLU	B	1181	10.653	24.601	21.881	1	80.88
3941	CD	GLU	B	1181	10.135	23.304	21.266	1	87.34
3942	OE1	GLU	B	1181	10.923	22.595	20.598	1	90.4
3943	OE2	GLU	B	1181	8.938	22.987	21.46	1	88.92
3944	N	MET	B	1182	11.172	26.719	25.65	1	67.19
3945	CA	MET	B	1182	10.629	26.837	27.005	1	64.01
3946	C	MET	B	1182	9.095	26.854	27.064	1	60.76
3947	O	MET	B	1182	8.434	26.902	26.039	1	63.29
3948	CB	MET	B	1182	11.226	28.075	27.689	1	60.43
3949	CG	MET	B	1182	12.73	27.982	27.816	1	57.06
3950	SD	MET	B	1182	13.528	29.48	28.35	1	56.31
3951	CE	MET	B	1182	13.742	30.289	26.803	1	57.39
3952	N	TPO	B	1183	8.541	26.8	28.27	1	57.45
3953	CA	TPO	B	1183	7.098	26.799	28.461	1	57.48
3954	CB	TPO	B	1183	6.738	26.374	29.934	1	57.7
3955	CG2	TPO	B	1183	5.351	26.891	30.377	1	58.92
3956	OG1	TPO	B	1183	7.748	26.891	30.753	1	54.66
3957	P	TPO	B	1183	8.733	25.956	31.446	1	55.58
3958	O1P	TPO	B	1183	10.016	25.979	30.672	1	44.08
3959	O2P	TPO	B	1183	8.095	24.586	31.429	1	54.5
3960	O3P	TPO	B	1183	8.998	26.512	32.775	1	47.5
3961	C	TPO	B	1183	6.492	28.142	27.99	1	57.58
3962	O	TPO	B	1183	7.073	29.217	28.188	1	56.01
3963	N	GLY	B	1184	5.358	28.037	27.295	1	55.43
3964	CA	GLY	B	1184	4.683	29.179	26.707	1	52.19
3965	C	GLY	B	1184	4.124	30.308	27.537	1	54.15
3966	O	GLY	B	1184	4.546	31.465	27.368	1	55.41
3967	N	PTR	B	1185	3.135	30.016	28.38	1	52.22
3968	CA	PTR	B	1185	2.522	31.071	29.187	1	51.44
3969	C	PTR	B	1185	3.404	31.475	30.376	1	50.95
3970	O	PTR	B	1185	3.3	30.894	31.46	1	51.63
3971	CB	PTR	B	1185	1.129	30.637	29.648	1	50.17
3972	CG	PTR	B	1185	0.187	31.812	29.599	1	49.77
3973	CD1	PTR	B	1185	-0.641	32.039	30.723	1	51.36
3974	CD2	PTR	B	1185	0.138	32.682	28.503	1	50.95
3975	CE1	PTR	B	1185	-1.527	33.122	30.776	1	48.41
3976	CE2	PTR	B	1185	-0.754	33.778	28.565	1	50.34

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
3977	CZ	PTR	B	1185	-1.578	33.986	29.696	1	49.75
3978	OH	PTR	B	1185	-2.507	34.994	29.665	1	52.59
3979	P	PTR	B	1185	-2.638	36.081	30.757	1	55.23
3980	O1P	PTR	B	1185	-1.812	35.798	31.921	1	60.66
3981	O2P	PTR	B	1185	-4.028	36.033	31.2	1	55.96
3982	O3P	PTR	B	1185	-2.363	37.376	30.187	1	55.33
3983	N	VAL	B	1186	4.27	32.468	30.162	1	47.01
3984	CA	VAL	B	1186	5.18	32.936	31.2	1	43.17
3985	C	VAL	B	1186	5.185	34.455	31.307	1	41.43
3986	O	VAL	B	1186	4.803	35.126	30.375	1	44.65
3987	CB	VAL	B	1186	6.612	32.412	30.933	1	45.49
3988	CG1	VAL	B	1186	6.614	30.873	30.884	1	46.53
3989	CG2	VAL	B	1186	7.156	32.969	29.63	1	42.01
3990	N	VAL	B	1187	5.645	34.99	32.437	1	43.35
3991	CA	VAL	B	1187	5.694	36.448	32.719	1	41.61
3992	C	VAL	B	1187	4.305	37.012	32.991	1	41.24
3993	O	VAL	B	1187	3.343	36.61	32.357	1	44.73
3994	CB	VAL	B	1187	6.28	37.298	31.573	1	36.39
3995	CG1	VAL	B	1187	6.545	38.697	32.074	1	37.09
3996	CG2	VAL	B	1187	7.552	36.705	31.04	1	41.27
3997	N	THR	B	1188	4.193	37.932	33.942	1	44.12
3998	CA	THR	B	1188	2.9	38.547	34.239	1	42.9
3999	C	THR	B	1188	2.558	39.438	33.068	1	42.74
4000	O	THR	B	1188	3.414	40.187	32.586	1	42.98
4001	CB	THR	B	1188	2.941	39.365	35.521	1	44.42
4002	OG1	THR	B	1188	3.198	38.49	36.639	1	44.96
4003	CG2	THR	B	1188	1.611	40.092	35.724	1	41.85
4004	N	ARG	B	1189	1.317	39.33	32.596	1	46.74
4005	CA	ARG	B	1189	0.83	40.083	31.423	1	48.63
4006	C	ARG	B	1189	1.354	41.508	31.138	1	45.25
4007	O	ARG	B	1189	1.954	41.739	30.1	1	46.29
4008	CB	ARG	B	1189	-0.708	40.08	31.367	1	48.77
4009	CG	ARG	B	1189	-1.259	40.65	30.054	1	50.27
4010	CD	ARG	B	1189	-2.764	40.895	30.08	1	48.77
4011	NE	ARG	B	1189	-3.498	39.663	30.322	1	47.77
4012	CZ	ARG	B	1189	-4.501	39.549	31.181	1	48.48
4013	NH1	ARG	B	1189	-4.904	40.603	31.887	1	50.17
4014	NH2	ARG	B	1189	-5.089	38.377	31.35	1	45.66
4015	N	TRP	B	1190	1.145	42.453	32.039	1	41.32
4016	CA	TRP	B	1190	1.596	43.809	31.762	1	48.65
4017	C	TRP	B	1190	3.102	43.966	31.58	1	46.42
4018	O	TRP	B	1190	3.558	44.979	31.072	1	46.22
4019	CB	TRP	B	1190	1.053	44.813	32.808	1	53.47
4020	CG	TRP	B	1190	-0.461	44.8	32.938	1	60.03
4021	CD1	TRP	B	1190	-1.354	44.345	32.01	1	63.94
4022	CD2	TRP	B	1190	-1.244	45.197	34.076	1	64.5
4023	NE1	TRP	B	1190	-2.636	44.422	32.499	1	66.54
4024	CE2	TRP	B	1190	-2.596	44.943	33.764	1	67.44
4025	CE3	TRP	B	1190	-0.931	45.734	35.331	1	69.36
4026	CZ2	TRP	B	1190	-3.637	45.207	34.663	1	68.28
4027	CZ3	TRP	B	1190	-1.968	45.995	36.226	1	68.93
4028	CH2	TRP	B	1190	-3.303	45.73	35.883	1	70
4029	N	TYR	B	1191	3.865	42.94	31.922	1	44.91
4030	CA	TYR	B	1191	5.311	43.014	31.792	1	44.62
4031	C	TYR	B	1191	5.815	42.002	30.787	1	46.4-
4032	O	TYR	B	1191	7.015	41.881	30.531	1	49.89

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4033	CB	TYR	B	1191	5.96	42.814	33.162	1	45.67
4034	CG	TYR	B	1191	5.439	43.799	34.167	1	43.36
4035	CD1	TYR	B	1191	5.962	45.089	34.24	1	44.9
4036	CD2	TYR	B	1191	4.341	43.487	34.961	1	46.89
4037	CE1	TYR	B	1191	5.386	46.048	35.063	1	46.19
4038	CE2	TYR	B	1191	3.762	44.436	35.793	1	46.56
4039	CZ	TYR	B	1191	4.286	45.712	35.83	1	46.76
4040	OH	TYR	B	1191	3.685	46.663	36.611	1	52.39
4041	N	ARG	B	1192	4.865	41.316	30.175	1	47.02
4042	CA	ARG	B	1192	5.15	40.305	29.183	1	44.82
4043	C	ARG	B	1192	5.523	40.921	27.83	1	46
4044	O	ARG	B	1192	4.841	41.812	27.326	1	48.59
4045	CB	ARG	B	1192	3.937	39.389	29.057	1	39.1
4046	CG	ARG	B	1192	4.123	38.28	28.102	1	39.95
4047	CD	ARG	B	1192	3.436	37.072	28.632	1	43.68
4048	NE	ARG	B	1192	2	37.133	28.453	1	47.31
4049	CZ	ARG	B	1192	1.121	36.801	29.384	1	48.78
4050	NH1	ARG	B	1192	1.539	36.401	30.566	1	44.85
4051	NH2	ARG	B	1192	-0.174	36.817	29.104	1	53.73
4052	N	ALA	B	1193	6.631	40.454	27.264	1	45.8
4053	CA	ALA	B	1193	7.098	40.932	25.983	1	42.03
4054	C	ALA	B	1193	6.251	40.291	24.897	1	44.54
4055	O	ALA	B	1193	5.815	39.139	25.025	1	46.29
4056	CB	ALA	B	1193	8.527	40.567	25.803	1	40.43
4057	N	PRO	B	1194	6.044	41.009	23.786	1	42.28
4058	CA	PRO	B	1194	5.243	40.493	22.679	1	42.12
4059	C	PRO	B	1194	5.642	39.107	22.143	1	44.43
4060	O	PRO	B	1194	4.773	38.267	21.841	1	44.4
4061	CB	PRO	B	1194	5.405	41.575	21.618	1	40.5
4062	CG	PRO	B	1194	6.706	42.209	21.963	1	41.2
4063	CD	PRO	B	1194	6.632	42.31	23.44	1	38.61
4064	N	GLU	B	1195	6.942	38.845	22.051	1	41.59
4065	CA	GLU	B	1195	7.349	37.564	21.512	1	41.49
4066	C	GLU	B	1195	6.949	36.356	22.333	1	41.11
4067	O	GLU	B	1195	6.965	35.247	21.817	1	41.88
4068	CB	GLU	B	1195	8.827	37.521	21.164	1	42.13
4069	CG	GLU	B	1195	9.752	37.453	22.326	1	46.22
4070	CD	GLU	B	1195	10.016	38.791	22.979	1	47.44
4071	OE1	GLU	B	1195	9.548	39.851	22.489	1	46.07
4072	OE2	GLU	B	1195	10.715	38.756	24.004	1	44.98
4073	N	VAL	B	1196	6.546	36.554	23.588	1	43.14
4074	CA	VAL	B	1196	6.104	35.42	24.405	1	42.76
4075	C	VAL	B	1196	4.893	34.8	23.714	1	48.78
4076	O	VAL	B	1196	4.632	33.599	23.836	1	49.71
4077	CB	VAL	B	1196	5.696	35.85	25.82	1	41.44
4078	CG1	VAL	B	1196	5.223	34.652	26.627	1	37.67
4079	CG2	VAL	B	1196	6.876	36.52	26.508	1	43.73
4080	N	ILE	B	1197	4.19	35.623	22.933	1	51.47
4081	CA	ILE	B	1197	3.007	35.176	22.214	1	48.3
4082	C	ILE	B	1197	3.227	35.039	20.719	1	45.29
4083	O	ILE	B	1197	2.86	34.021	20.145	1	42.3
4084	CB	ILE	B	1197	1.809	36.087	22.54	1	50.42
4085	CG1	ILE	B	1197	1.466	35.909	24.015	1	47.59
4086	CG2	ILE	B	1197	0.593	35.742	21.672	1	49.15
4087	CD1	ILE	B	1197	0.372	36.762	24.447	1	51.83
4088	N	LEU	B	1198	3.849	36.039	20.1	1	44.39

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4089	CA	LEU	B	1198	4.104	35.978	18.665	1	47.5
4090	C	LEU	B	1198	5.068	34.848	18.371	1	51.67
4091	O	LEU	B	1198	4.983	34.199	17.321	1	55.4
4092	CB	LEU	B	1198	4.677	37.298	18.137	1	45.4
4093	CG	LEU	B	1198	3.763	38.513	18.347	1	47.12
4094	CD1	LEU	B	1198	4.272	39.714	17.583	1	38.91
4095	CD2	LEU	B	1198	2.348	38.162	17.924	1	44.07
4096	N	ASN	B	1199	5.978	34.608	19.312	1	52.22
4097	CA	ASN	B	1199	6.964	33.552	19.166	1	52.73
4098	C	ASN	B	1199	6.79	32.502	20.251	1	53.9
4099	O	ASN	B	1199	7.739	32.176	20.959	1	55.29
4100	CB	ASN	B	1199	8.37	34.136	19.238	1	54.27
4101	CG	ASN	B	1199	9.428	33.161	18.776	1	53.46
4102	OD1	ASN	B	1199	9.13	32.006	18.464	1	47.79
4103	ND2	ASN	B	1199	10.672	33.626	18.717	1	50.82
4104	N	TRP	B	1200	5.578	31.966	20.359	1	54.16
4105	CA	TRP	B	1200	5.236	30.941	21.337	1	54.29
4106	C	TRP	B	1200	6.371	29.938	21.568	1	55.78
4107	O	TRP	B	1200	6.907	29.371	20.614	1	56.65
4108	CB	TRP	B	1200	3.992	30.194	20.859	1	53.09
4109	CG	TRP	B	1200	3.419	29.254	21.855	1	53.23
4110	CD1	TRP	B	1200	3.405	27.884	21.788	1	55.49
4111	CD2	TRP	B	1200	2.728	29.605	23.054	1	52.08
4112	NE1	TRP	B	1200	2.733	27.362	22.877	1	54.45
4113	CE2	TRP	B	1200	2.308	28.397	23.668	1	51.15
4114	CE3	TRP	B	1200	2.414	30.825	23.673	1	51.63
4115	CZ2	TRP	B	1200	1.593	28.377	24.865	1	50.67
4116	CZ3	TRP	B	1200	1.706	30.809	24.856	1	48.87
4117	CH2	TRP	B	1200	1.3	29.588	25.444	1	51.53
4118	N	MET	B	1201	6.77	29.804	22.835	1	55.53
4119	CA	MET	B	1201	7.822	28.887	23.304	1	52.33
4120	C	MET	B	1201	9.266	29.122	22.873	1	52.99
4121	O	MET	B	1201	10.136	28.319	23.216	1	53.52
4122	CB	MET	B	1201	7.448	27.433	23.007	1	48.18
4123	CG	MET	B	1201	6.198	26.983	23.704	1	52.88
4124	SD	MET	B	1201	5.807	25.24	23.47	1	59.31
4125	CE	MET	B	1201	4.293	25.095	24.49	1	52.9
4126	N	ARG	B	1202	9.553	30.213	22.166	1	49.95
4127	CA	ARG	B	1202	10.927	30.433	21.719	1	48.96
4128	C	ARG	B	1202	11.506	31.808	22.016	1	49.58
4129	O	ARG	B	1202	12.319	32.329	21.254	1	50.5
4130	CB	ARG	B	1202	11.063	30.111	20.231	1	51.19
4131	CG	ARG	B	1202	10.613	28.697	19.868	1	55.45
4132	CD	ARG	B	1202	10.812	28.416	18.388	1	56.08
4133	NE	ARG	B	1202	10.561	27.016	18.069	1	58.32
4134	CZ	ARG	B	1202	9.41	26.548	17.604	1	60.02
4135	NH1	ARG	B	1202	8.396	27.376	17.399	1	59.12
4136	NH2	ARG	B	1202	9.275	25.249	17.347	1	59.14
4137	N	TYR	B	1203	11.075	32.401	23.119	1	48.73
4138	CA	TYR	B	1203	11.584	33.698	23.544	1	51.01
4139	C	TYR	B	1203	12.92	33.455	24.252	1	52.73
4140	O	TYR	B	1203	13.288	32.312	24.525	1	52.4
4141	CB	TYR	B	1203	10.619	34.336	24.534	1	50.36
4142	CG	TYR	B	1203	10.247	33.392	25.653	1	49.96
4143	CD1	TYR	B	1203	9.194	32.5	25.505	1	47.63
4144	CD2	TYR	B	1203	10.985	33.35	26.849	1	52.8

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4145	CE1	TYR	B	1203	8.882	31.578	26.51	1	50.33
4146	CE2	TYR	B	1203	10.669	32.424	27.868	1	47.24
4147	CZ	TYR	B	1203	9.618	31.553	27.674	1	47.25
4148	OH	TYR	B	1203	9.27	30.656	28.638	1	55.01
4149	N	THR	B	1204	13.631	34.525	24.585	1	53.03
4150	CA	THR	B	1204	14.908	34.37	25.253	1	53.27
4151	C	THR	B	1204	15.014	35.208	26.507	1	52.16
4152	O	THR	B	1204	14.031	35.755	26.997	1	53.18
4153	CB	THR	B	1204	16.104	34.71	24.33	1	54.94
4154	OG1	THR	B	1204	16.035	36.083	23.922	1	54.05
4155	CG2	THR	B	1204	16.12	33.805	23.119	1	55.19
4156	N	GLN	B	1205	16.227	35.291	27.028	1	50.17
4157	CA	GLN	B	1205	16.487	36.052	28.22	1	48.17
4158	C	GLN	B	1205	16.165	37.505	27.982	1	46.85
4159	O	GLN	B	1205	16.147	38.288	28.918	1	48.64
4160	CB	GLN	B	1205	17.948	35.928	28.607	1	50.3
4161	CG	GLN	B	1205	18.464	34.511	28.626	1	56.04
4162	CD	GLN	B	1205	19.92	34.468	29.005	1	57.7
4163	OE1	GLN	B	1205	20.753	35.119	28.367	1	63.39
4164	NE2	GLN	B	1205	20.235	33.745	30.075	1	55.88
4165	N	THR	B	1206	15.959	37.894	26.732	1	46.01
4166	CA	THR	B	1206	15.631	39.287	26.472	1	46.63
4167	C	THR	B	1206	14.243	39.658	26.978	1	44.63
4168	O	THR	B	1206	13.938	40.852	27.125	1	44.04
4169	CB	THR	B	1206	15.734	39.655	24.998	1	47.86
4170	OG1	THR	B	1206	15.217	38.583	24.208	1	49.04
4171	CG2	THR	B	1206	17.172	39.971	24.62	1	47.78
4172	N	VAL	B	1207	13.412	38.653	27.259	1	38.86
4173	CA	VAL	B	1207	12.074	38.944	27.756	1	37.69
4174	C	VAL	B	1207	12.178	39.641	29.088	1	36.51
4175	O	VAL	B	1207	11.324	40.445	29.415	1	39.99
4176	CB	VAL	B	1207	11.181	37.701	27.914	1	36.07
4177	CG1	VAL	B	1207	11.301	36.835	26.716	1	38.1
4178	CG2	VAL	B	1207	11.517	36.941	29.17	1	33.88
4179	N	ASP	B	1208	13.234	39.34	29.841	1	36.82
4180	CA	ASP	B	1208	13.453	39.964	31.144	1	38.33
4181	C	ASP	B	1208	13.838	41.421	30.931	1	38.75
4182	O	ASP	B	1208	13.662	42.243	31.818	1	42.78
4183	CB	ASP	B	1208	14.567	39.243	31.933	1	40.62
4184	CG	ASP	B	1208	14.18	37.822	32.362	1	47.14
4185	OD1	ASP	B	1208	12.971	37.558	32.556	1	51.31
4186	OD2	ASP	B	1208	15.091	36.975	32.54	1	47.58
4187	N	ILE	B	1209	14.415	41.736	29.772	1	40.72
4188	CA	ILE	B	1209	14.795	43.118	29.488	1	44.12
4189	C	ILE	B	1209	13.523	43.88	29.167	1	43.61
4190	O	ILE	B	1209	13.395	45.046	29.52	1	44.66
4191	CB	ILE	B	1209	15.803	43.233	28.321	1	46.12
4192	CG1	ILE	B	1209	17.142	42.634	28.744	1	46.44
4193	CG2	ILE	B	1209	16.025	44.709	27.951	1	46.63
4194	CD1	ILE	B	1209	17.735	43.33	29.925	1	47.31
4195	N	TRP	B	1210	12.569	43.201	28.53	1	42.85
4196	CA	TRP	B	1210	11.303	43.82	28.216	1	43.23
4197	C	TRP	B	1210	10.684	44.24	29.538	1	47.23
4198	O	TRP	B	1210	10.439	45.436	29.765	1	50.13
4199	CB	TRP	B	1210	10.375	42.86	27.472	1	44.24
4200	CG	TRP	B	1210	9.059	43.522	27.091	1	46.15

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4201	CD1	TRP	B	1210	7.934	43.604	27.859	1	47.45
4202	CD2	TRP	B	1210	8.784	44.275	25.904	1	43.99
4203	NE1	TRP	B	1210	6.986	44.37	27.235	1	47.93
4204	CE2	TRP	B	1210	7.482	44.794	26.032	1	48.37
4205	CE3	TRP	B	1210	9.514	44.566	24.749	1	45.13
4206	CZ2	TRP	B	1210	6.892	45.597	25.043	1	48.76
4207	CZ3	TRP	B	1210	8.929	45.356	23.769	1	45.48
4208	CH2	TRP	B	1210	7.632	45.863	23.922	1	45.3
4209	N	SER	B	1211	10.491	43.265	30.428	1	45.87
4210	CA	SER	B	1211	9.929	43.521	31.752	1	43.19
4211	C	SER	B	1211	10.64	44.688	32.436	1	42.84
4212	O	SER	B	1211	9.997	45.594	32.962	1	47.32
4213	CB	SER	B	1211	10.013	42.268	32.62	1	41.32
4214	OG	SER	B	1211	9.246	41.22	32.055	1	44.51
4215	N	VAL	B	1212	11.963	44.703	32.406	1	38.65
4216	CA	VAL	B	1212	12.675	45.821	33.03	1	36.73
4217	C	VAL	B	1212	12.3	47.176	32.381	1	35.46
4218	O	VAL	B	1212	12.285	48.215	33.041	1	31.21
4219	CB	VAL	B	1212	14.212	45.6	32.994	1	33.77
4220	CG1	VAL	B	1212	14.938	46.829	33.476	1	26.48
4221	CG2	VAL	B	1212	14.577	44.417	33.893	1	33.6
4222	N	GLY	B	1213	11.983	47.15	31.09	1	33.45
4223	CA	GLY	B	1213	11.618	48.379	30.408	1	37.91
4224	C	GLY	B	1213	10.272	48.894	30.88	1	40.63
4225	O	GLY	B	1213	10.111	50.078	31.154	1	42.93
4226	N	CYS	B	1214	9.296	47.996	30.95	1	40.03
4227	CA	CYS	B	1214	7.974	48.342	31.414	1	38.79
4228	C	CYS	B	1214	8.087	48.81	32.856	1	40.72
4229	O	CYS	B	1214	7.409	49.744	33.278	1	44.91
4230	CB	CYS	B	1214	7.077	47.111	31.376	1	41.67
4231	SG	CYS	B	1214	6.855	46.384	29.756	1	44.47
4232	N	ILE	B	1215	8.948	48.155	33.618	1	39.23
4233	CA	ILE	B	1215	9.11	48.518	35.019	1	39.92
4234	C	ILE	B	1215	9.77	49.895	35.114	1	39.91
4235	O	ILE	B	1215	9.287	50.756	35.826	1	44.16
4236	CB	ILE	B	1215	9.92	47.443	35.818	1	31.4
4237	CG1	ILE	B	1215	9.236	46.068	35.736	1	34.39
4238	CG2	ILE	B	1215	9.971	47.809	37.246	1	31.38
4239	CD1	ILE	B	1215	10.017	44.906	36.35	1	20.27
4240	N	MET	B	1216	10.844	50.115	34.375	1	40.74
4241	CA	MET	B	1216	11.52	51.411	34.428	1	45.73
4242	C	MET	B	1216	10.573	52.508	33.94	1	47.65
4243	O	MET	B	1216	10.555	53.611	34.478	1	47.43
4244	CB	MET	B	1216	12.776	51.415	33.556	1	44.71
4245	CG	MET	B	1216	13.646	52.632	33.797	1	48.1
4246	SD	MET	B	1216	14.799	53.015	32.451	1	49.17
4247	CE	MET	B	1216	15.345	54.577	33.017	1	51.17
4248	N	ALA	B	1217	9.768	52.174	32.934	1	48.37
4249	CA	ALA	B	1217	8.818	53.102	32.358	1	48.15
4250	C	ALA	B	1217	7.761	53.474	33.387	1	51.73
4251	O	ALA	B	1217	7.374	54.639	33.507	1	54.48
4252	CB	ALA	B	1217	8.173	52.479	31.149	1	44.59
4253	N	GLU	B	1218	7.332	52.478	34.158	1	52.41
4254	CA	GLU	B	1218	6.318	52.675	35.182	1	50.52
4255	C	GLU	B	1218	6.837	53.53	36.327	1	50.04
4256	O	GLU	B	1218	6.101	54.324	36.889	1	51.73

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4257	CB	GLU	B	1218	5.835	51.329	35.717	1	49.08
4258	CG	GLU	B	1218	4.569	51.44	36.529	1	47.77
4259	CD	GLU	B	1218	4.022	50.097	36.961	1	48.84
4260	OE1	GLU	B	1218	4.236	49.088	36.262	1	42.73
4261	OE2	GLU	B	1218	3.354	50.055	38.01	1	52.26
4262	N	MET	B	1219	8.095	53.343	36.699	1	49.38
4263	CA	MET	B	1219	8.661	54.13	37.774	1	50.62
4264	C	MET	B	1219	8.607	55.613	37.403	1	54.4
4265	O	MET	B	1219	8.24	56.455	38.228	1	56.92
4266	CB	MET	B	1219	10.11	53.72	38.032	1	45.89
4267	CG	MET	B	1219	10.271	52.373	38.645	1	42.73
4268	SD	MET	B	1219	11.979	51.838	38.549	1	43.34
4269	CE	MET	B	1219	12.61	52.259	40.04	1	38.93
4270	N	ILE	B	1220	8.925	55.916	36.147	1	55.54
4271	CA	ILE	B	1220	8.945	57.291	35.662	1	58.01
4272	C	ILE	B	1220	7.569	57.967	35.515	1	60
4273	O	ILE	B	1220	7.362	59.084	36.01	1	61.51
4274	CB	ILE	B	1220	9.661	57.378	34.308	1	57.72
4275	CG1	ILE	B	1220	11.024	56.706	34.388	1	52.49
4276	CG2	ILE	B	1220	9.842	58.844	33.915	1	59.88
4277	CD1	ILE	B	1220	11.711	56.607	33.053	1	50.93
4278	N	THR	B	1221	6.657	57.308	34.798	1	58.95
4279	CA	THR	B	1221	5.322	57.835	34.564	1	56.6
4280	C	THR	B	1221	4.424	57.702	35.765	1	58.55
4281	O	THR	B	1221	3.714	58.638	36.113	1	64.3
4282	CB	THR	B	1221	4.614	57.113	33.425	1	57.49
4283	OG1	THR	B	1221	4.306	55.778	33.838	1	56.17
4284	CG2	THR	B	1221	5.478	57.101	32.156	1	58.21
4285	N	GLY	B	1222	4.423	56.522	36.371	1	58.22
4286	CA	GLY	B	1222	3.575	56.277	37.527	1	56.24
4287	C	GLY	B	1222	2.405	55.392	37.142	1	55.43
4288	O	GLY	B	1222	1.722	54.827	38	1	54.04
4289	N	LYS	B	1223	2.21	55.25	35.836	1	55.15
4290	CA	LYS	B	1223	1.14	54.435	35.287	1	57.33
4291	C	LYS	B	1223	1.728	53.179	34.653	1	57.5
4292	O	LYS	B	1223	2.881	53.171	34.245	1	58.38
4293	CB	LYS	B	1223	0.364	55.241	34.224	1	55.24
4294	N	THR	B	1224	0.936	52.114	34.597	1	57.62
4295	CA	THR	B	1224	1.36	50.872	33.969	1	56.46
4296	C	THR	B	1224	1.478	51.199	32.486	1	58.78
4297	O	THR	B	1224	0.557	51.793	31.908	1	61.77
4298	CB	THR	B	1224	0.305	49.786	34.185	1	55.89
4299	OG1	THR	B	1224	0.174	49.546	35.593	1	57.63
4300	CG2	THR	B	1224	0.681	48.497	33.469	1	54.77
4301	N	LEU	B	1225	2.606	50.834	31.877	1	57.8
4302	CA	LEU	B	1225	2.853	51.133	30.467	1	55.6
4303	C	LEU	B	1225	1.908	50.463	29.478	1	53.47
4304	O	LEU	B	1225	1.3	51.131	28.663	1	54.96
4305	CB	LEU	B	1225	4.311	50.849	30.097	1	54.83
4306	CG	LEU	B	1225	4.717	51.246	28.676	1	56.4
4307	CD1	LEU	B	1225	4.379	52.7	28.434	1	56.41
4308	CD2	LEU	B	1225	6.196	51.004	28.464	1	55.43
4309	N	PHE	B	1226	1.79	49.148	29.538	1	52.6
4310	CA	PHE	B	1226	0.901	48.444	28.619	1	54.7
4311	C	PHE	B	1226	-0.112	47.622	29.436	1	57.14
4312	O	PHE	B	1226	0.115	46.441	29.711	1	58.96

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4313	CB	PHE	B	1226	1.7	47.523	27.663	1	50.21
4314	CG	PHE	B	1226	2.827	48.218	26.914	1	48.07
4315	CD1	PHE	B	1226	2.588	49.345	26.136	1	47.09
4316	CD2	PHE	B	1226	4.136	47.748	27.009	1	46.21
4317	CE1	PHE	B	1226	3.633	49.99	25.474	1	45.24
4318	CE2	PHE	B	1226	5.182	48.389	26.35	1	44.35
4319	CZ	PHE	B	1226	4.927	49.511	25.585	1	44.76
4320	N	LYS	B	1227	-1.213	48.253	29.841	1	57.52
4321	CA	LYS	B	1227	-2.229	47.564	30.627	1	59.66
4322	C	LYS	B	1227	-3.262	46.911	29.711	1	61.37
4323	O	LYS	B	1227	-4.25	47.535	29.346	1	66.75
4324	CB	LYS	B	1227	-2.907	48.544	31.599	1	59.39
4325	N	GLY	B	1228	-3.026	45.666	29.312	1	58.81
4326	CA	GLY	B	1228	-3.969	45.006	28.429	1	58.75
4327	C	GLY	B	1228	-4.983	44.165	29.168	1	59.74
4328	O	GLY	B	1228	-4.687	43.673	30.254	1	60.68
4329	N	SER	B	1229	-6.148	43.944	28.559	1	60.74
4330	CA	SER	B	1229	-7.206	43.153	29.196	1	62.57
4331	C	SER	B	1229	-6.961	41.647	29.164	1	61.96
4332	O	SER	B	1229	-7.304	40.947	30.122	1	60.7
4333	CB	SER	B	1229	-8.585	43.495	28.622	1	63.3
4334	OG	SER	B	1229	-8.71	43.085	27.275	1	66.67
4335	N	ASP	B	1230	-6.411	41.148	28.058	1	61.15
4336	CA	ASP	B	1230	-6.088	39.724	27.93	1	62.19
4337	C	ASP	B	1230	-4.755	39.597	27.216	1	60.17
4338	O	ASP	B	1230	-4.221	40.601	26.738	1	60.7
4339	CB	ASP	B	1230	-7.196	38.919	27.22	1	66.13
4340	CG	ASP	B	1230	-7.542	39.459	25.835	1	71.54
4341	OD1	ASP	B	1230	-8.415	40.346	25.744	1	73.7
4342	OD2	ASP	B	1230	-6.968	38.977	24.834	1	74.52
4343	N	HIS	B	1231	-4.219	38.38	27.128	1	59.02
4344	CA	HIS	B	1231	-2.913	38.189	26.494	1	58.04
4345	C	HIS	B	1231	-2.807	38.689	25.069	1	57.96
4346	O	HIS	B	1231	-1.771	39.219	24.671	1	58.46
4347	CB	HIS	B	1231	-2.429	36.747	26.602	1	55.94
4348	CG	HIS	B	1231	-3.263	35.763	25.851	1	56.86
4349	ND1	HIS	B	1231	-4.4	35.196	26.383	1	56.73
4350	CD2	HIS	B	1231	-3.073	35.17	24.652	1	57.29
4351	CE1	HIS	B	1231	-4.87	34.29	25.543	1	58.59
4352	NE2	HIS	B	1231	-4.083	34.255	24.484	1	59.01
4353	N	LEU	B	1232	-3.885	38.543	24.308	1	58.32
4354	CA	LEU	B	1232	-3.911	39.027	22.941	1	54.34
4355	C	LEU	B	1232	-4.072	40.539	22.947	1	54.1
4356	O	LEU	B	1232	-3.415	41.241	22.183	1	56.3
4357	CB	LEU	B	1232	-5.064	38.405	22.182	1	55.14
4358	CG	LEU	B	1232	-4.998	36.905	21.922	1	57.44
4359	CD1	LEU	B	1232	-6.223	36.494	21.117	1	57.88
4360	CD2	LEU	B	1232	-3.715	36.556	21.162	1	56.89
4361	N	ASP	B	1233	-4.927	41.047	23.826	1	51.61
4362	CA	ASP	B	1233	-5.149	42.486	23.896	1	52.19
4363	C	ASP	B	1233	-3.875	43.223	24.331	1	52.92
4364	O	ASP	B	1233	-3.689	44.419	24.033	1	50.75
4365	CB	ASP	B	1233	-6.303	42.803	24.849	1	50.34
4366	CG	ASP	B	1233	-6.653	44.28	24.864	1	52.85
4367	OD1	ASP	B	1233	-6.945	44.836	23.79	1	52.13
4368	OD2	ASP	B	1233	-6.629	44.892	25.949	1	56.19

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4369	N	GLN	B	1234	-3.007	42.498	25.04	1	50.31
4370	CA	GLN	B	1234	-1.744	43.053	25.517	1	50.45
4371	C	GLN	B	1234	-0.887	43.389	24.293	1	50.93
4372	O	GLN	B	1234	-0.176	44.407	24.261	1	51.59
4373	CB	GLN	B	1234	-1.041	42.04	26.421	1	45.74
4374	CG	GLN	B	1234	0.279	42.508	26.982	1	46.08
4375	CD	GLN	B	1234	0.134	43.546	28.077	1	46.94
4376	OE1	GLN	B	1234	-0.707	43.407	28.943	1	46.68
4377	NE2	GLN	B	1234	0.989	44.578	28.062	1	46.35
4378	N	LEU	B	1235	-0.977	42.539	23.274	1	48.65
4379	CA	LEU	B	1235	-0.237	42.782	22.055	1	48.98
4380	C	LEU	B	1235	-0.691	44.123	21.516	1	52.23
4381	O	LEU	B	1235	0.142	45.004	21.303	1	53.03
4382	CB	LEU	B	1235	-0.488	41.68	21.036	1	45.58
4383	CG	LEU	B	1235	0.095	40.327	21.433	1	44.53
4384	CD1	LEU	B	1235	-0.092	39.335	20.314	1	43.17
4385	CD2	LEU	B	1235	1.581	40.49	21.733	1	46.57
4386	N	LYS	B	1236	-2.012	44.319	21.416	1	54.96
4387	CA	LYS	B	1236	-2.557	45.585	20.909	1	54.89
4388	C	LYS	B	1236	-2.069	46.787	21.708	1	54.06
4389	O	LYS	B	1236	-1.66	47.797	21.131	1	54.93
4390	CB	LYS	B	1236	-4.095	45.581	20.841	1	57.59
4391	CG	LYS	B	1236	-4.71	46.952	20.449	1	62.19
4392	CD	LYS	B	1236	-6.05	46.867	19.682	1	67.51
4393	CE	LYS	B	1236	-7.204	46.304	20.517	1	71.25
4394	NZ	LYS	B	1236	-8.498	46.253	19.768	1	69.27
4395	N	GLU	B	1237	-2.096	46.688	23.03	1	52.2
4396	CA	GLU	B	1237	-1.63	47.803	23.831	1	53.59
4397	C	GLU	B	1237	-0.178	48.115	23.526	1	55.73
4398	O	GLU	B	1237	0.175	49.275	23.364	1	59.93
4399	CB	GLU	B	1237	-1.819	47.55	25.324	1	54.74
4400	CG	GLU	B	1237	-3.207	47.909	25.861	1	54.47
4401	CD	GLU	B	1237	-3.65	49.307	25.47	1	53.34
4402	OE1	GLU	B	1237	-2.963	50.291	25.822	1	53.72
4403	OE2	GLU	B	1237	-4.687	49.412	24.791	1	51.62
4404	N	ILE	B	1238	0.652	47.08	23.389	1	56.11
4405	CA	ILE	B	1238	2.068	47.279	23.091	1	52.93
4406	C	ILE	B	1238	2.224	47.88	21.71	1	54.32
4407	O	ILE	B	1238	2.93	48.883	21.522	1	57.33
4408	CB	ILE	B	1238	2.833	45.961	23.119	1	50.68
4409	CG1	ILE	B	1238	2.839	45.397	24.538	1	46.12
4410	CG2	ILE	B	1238	4.23	46.155	22.553	1	45.3
4411	CD1	ILE	B	1238	3.235	43.941	24.621	1	42.78
4412	N	MET	B	1239	1.535	47.273	20.754	1	51.63
4413	CA	MET	B	1239	1.587	47.714	19.374	1	53.66
4414	C	MET	B	1239	1.216	49.18	19.217	1	53.7
4415	O	MET	B	1239	1.804	49.873	18.397	1	53.08
4416	CB	MET	B	1239	0.655	46.866	18.515	1	57.16
4417	CG	MET	B	1239	0.845	45.359	18.634	1	58.29
4418	SD	MET	B	1239	2.149	44.69	17.65	1	56.59
4419	CE	MET	B	1239	2.394	43.102	18.409	1	57.01
4420	N	LYS	B	1240	0.255	49.659	20.008	1	53.9
4421	CA	LYS	B	1240	-0.16	51.05	19.913	1	53.89
4422	C	LYS	B	1240	1.035	51.977	20.172	1	56.36
4423	O	LYS	B	1240	1.06	53.122	19.715	1	57.18
4424	CB	LYS	B	1240	-1.322	51.339	20.876	1	47.38

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4425	N	VAL	B	1241	2.065	51.435	20.82	1	58.45
4426	CA	VAL	B	1241	3.263	52.195	21.135	1	59.79
4427	C	VAL	B	1241	4.454	51.881	20.248	1	60.04
4428	O	VAL	B	1241	5.123	52.791	19.746	1	59.07
4429	CB	VAL	B	1241	3.671	51.966	22.578	1	60.53
4430	CG1	VAL	B	1241	4.93	52.746	22.909	1	62.42
4431	CG2	VAL	B	1241	2.547	52.379	23.483	1	63.8
4432	N	THR	B	1242	4.728	50.592	20.074	1	60.8
4433	CA	THR	B	1242	5.869	50.145	19.267	1	61.17
4434	C	THR	B	1242	5.535	49.966	17.795	1	61.01
4435	O	THR	B	1242	6.382	49.57	17.003	1	62.55
4436	CB	THR	B	1242	6.393	48.775	19.75	1	60.5
4437	OG1	THR	B	1242	5.483	47.75	19.343	1	54.06
4438	CG2	THR	B	1242	6.534	48.75	21.26	1	60.41
4439	N	GLY	B	1243	4.3	50.242	17.425	1	60.4
4440	CA	GLY	B	1243	3.921	50.032	16.05	1	60.89
4441	C	GLY	B	1243	3.718	48.541	15.864	1	61.31
4442	O	GLY	B	1243	4.048	47.741	16.746	1	60.67
4443	N	THR	B	1244	3.149	48.172	14.725	1	60.7
4444	CA	THR	B	1244	2.893	46.78	14.406	1	62.38
4445	C	THR	B	1244	3.947	46.309	13.419	1	64.56
4446	O	THR	B	1244	4.515	47.119	12.683	1	66.73
4447	CB	THR	B	1244	1.519	46.622	13.762	1	61.2
4448	OG1	THR	B	1244	1.395	47.563	12.691	1	62.03
4449	CG2	THR	B	1244	0.421	46.862	14.778	1	60.25
4450	N	PRO	B	1245	4.229	44.997	13.392	1	64.25
4451	CA	PRO	B	1245	5.222	44.421	12.486	1	66.03
4452	C	PRO	B	1245	4.69	44.482	11.056	1	67.01
4453	O	PRO	B	1245	3.521	44.798	10.839	1	67.35
4454	CB	PRO	B	1245	5.302	42.957	12.944	1	64.72
4455	CG	PRO	B	1245	4.745	42.951	14.292	1	64.39
4456	CD	PRO	B	1245	3.633	43.943	14.221	1	65.95
4457	N	PRO	B	1246	5.556	44.235	10.059	1	67.67
4458	CA	PRO	B	1246	5.106	44.261	8.668	1	67.56
4459	C	PRO	B	1246	4.065	43.167	8.418	1	68.23
4460	O	PRO	B	1246	4.116	42.086	9.01	1	65.68
4461	CB	PRO	B	1246	6.397	44.008	7.89	1	69.36
4462	CG	PRO	B	1246	7.288	43.3	8.877	1	69.55
4463	CD	PRO	B	1246	7.015	44.068	10.129	1	68.44
4464	N	ALA	B	1247	3.111	43.461	7.544	1	70.38
4465	CA	ALA	B	1247	2.037	42.526	7.227	1	71.09
4466	C	ALA	B	1247	2.508	41.169	6.707	1	71.05
4467	O	ALA	B	1247	1.873	40.15	6.976	1	70.69
4468	CB	ALA	B	1247	1.066	43.164	6.25	1	72.54
4469	N	GLU	B	1248	3.619	41.155	5.974	1	72.45
4470	CA	GLU	B	1248	4.161	39.908	5.425	1	72.67
4471	C	GLU	B	1248	4.692	38.986	6.522	1	70.87
4472	O	GLU	B	1248	4.681	37.764	6.373	1	69.68
4473	CB	GLU	B	1248	5.247	40.197	4.373	1	74.65
4474	CG	GLU	B	1248	6.514	40.891	4.886	1	76.7
4475	CD	GLU	B	1248	7.487	39.939	5.576	1	77.13
4476	OE1	GLU	B	1248	7.53	38.739	5.208	1	78.5
4477	OE2	GLU	B	1248	8.203	40.399	6.494	1	74.44
4478	N	PHE	B	1249	5.153	39.589	7.619	1	69.03
4479	CA	PHE	B	1249	5.681	38.845	8.76	1	65.7
4480	C	PHE	B	1249	4.565	38.116	9.479	1	62.87

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4481	O	PHE	B	1249	4.667	36.918	9.757	1	62.94
4482	CB	PHE	B	1249	6.387	39.781	9.755	1	64.18
4483	CG	PHE	B	1249	6.648	39.151	11.101	1	62.94
4484	CD1	PHE	B	1249	7.501	38.062	11.224	1	62.78
4485	CD2	PHE	B	1249	6.008	39.625	12.238	1	62.7
4486	CE1	PHE	B	1249	7.707	37.454	12.458	1	63.19
4487	CE2	PHE	B	1249	6.207	39.022	13.476	1	63.66
4488	CZ	PHE	B	1249	7.058	37.933	13.586	1	62.65
4489	N	VAL	B	1250	3.508	38.857	9.791	1	59.53
4490	CA	VAL	B	1250	2.377	38.294	10.501	1	58.75
4491	C	VAL	B	1250	1.651	37.229	9.687	1	58.44
4492	O	VAL	B	1250	0.964	36.378	10.242	1	58.71
4493	CB	VAL	B	1250	1.446	39.427	11.07	1	58.48
4494	CG1	VAL	B	1250	1.746	40.757	10.389	1	55.48
4495	CG2	VAL	B	1250	-0.031	39.053	10.968	1	54.45
4496	N	GLN	B	1251	1.894	37.231	8.382	1	60.21
4497	CA	GLN	B	1251	1.297	36.273	7.466	1	63.14
4498	C	GLN	B	1251	1.841	34.889	7.751	1	61.1
4499	O	GLN	B	1251	1.109	33.898	7.765	1	59.02
4500	CB	GLN	B	1251	1.68	36.639	6.034	1	70.12
4501	CG	GLN	B	1251	0.812	37.685	5.368	1	79.74
4502	CD	GLN	B	1251	-0.318	37.068	4.555	1	85.42
4503	OE1	GLN	B	1251	-0.951	36.085	4.972	1	88.27
4504	NE2	GLN	B	1251	-0.571	37.639	3.382	1	86.1
4505	N	ARG	B	1252	3.152	34.859	7.965	1	59.95
4506	CA	ARG	B	1252	3.921	33.648	8.21	1	57.86
4507	C	ARG	B	1252	3.999	33.181	9.656	1	57.82
4508	O	ARG	B	1252	4.692	32.207	9.941	1	57.09
4509	CB	ARG	B	1252	5.338	33.851	7.682	1	56.27
4510	CG	ARG	B	1252	5.388	34.332	6.263	1	52.49
4511	CD	ARG	B	1252	6.794	34.432	5.769	1	54.01
4512	NE	ARG	B	1252	7.457	35.651	6.211	1	58.28
4513	CZ	ARG	B	1252	8.648	35.676	6.8	1	61.18
4514	NH1	ARG	B	1252	9.301	34.539	7.03	1	63.42
4515	NH2	ARG	B	1252	9.217	36.836	7.097	1	59.41
4516	N	LEU	B	1253	3.336	33.886	10.571	1	55.24
4517	CA	LEU	B	1253	3.348	33.497	11.971	1	54.39
4518	C	LEU	B	1253	2.926	32.055	12.163	1	55.48
4519	O	LEU	B	1253	1.91	31.612	11.625	1	53.53
4520	CB	LEU	B	1253	2.449	34.402	12.796	1	53.23
4521	CG	LEU	B	1253	3.108	35.739	13.091	1	53.33
4522	CD1	LEU	B	1253	2.156	36.657	13.837	1	51.4
4523	CD2	LEU	B	1253	4.367	35.493	13.874	1	49.5
4524	N	GLN	B	1254	3.74	31.33	12.923	1	57.13
4525	CA	GLN	B	1254	3.516	29.927	13.221	1	60.09
4526	C	GLN	B	1254	2.269	29.742	14.074	1	62.32
4527	O	GLN	B	1254	1.442	28.869	13.804	1	62.17
4528	CB	GLN	B	1254	4.726	29.378	13.968	1	61.41
4529	CG	GLN	B	1254	5.259	28.079	13.42	1	68.18
4530	CD	GLN	B	1254	4.211	26.998	13.381	1	70.52
4531	OE1	GLN	B	1254	3.855	26.492	12.312	1	74.41
4532	NE2	GLN	B	1254	3.69	26.65	14.546	1	71.4
4533	N	SER	B	1255	2.152	30.563	15.115	1	65.61
4534	CA	SER	B	1255	1.011	30.507	16.022	1	68.55
4535	C	SER	B	1255	-0.249	30.996	15.327	1	69.94
4536	O	SER	B	1255	-0.306	32.14	14.876	1	70.72

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4537	CB	SER	B	1255	1.268	31.356	17.275	1	69.1
4538	OG	SER	B	1255	0.355	31.03	18.313	1	68.78
4539	N	ASP	B	1256	-1.238	30.109	15.204	1	70.64
4540	CA	ASP	B	1256	-2.51	30.454	14.575	1	70.68
4541	C	ASP	B	1256	-3.187	31.581	15.353	1	70.67
4542	O	ASP	B	1256	-3.499	32.634	14.792	1	69.86
4543	CB	ASP	B	1256	-3.43	29.231	14.505	1	71.75
4544	CG	ASP	B	1256	-3.024	28.242	13.41	1	74.47
4545	OD1	ASP	B	1256	-1.945	28.417	12.805	1	74.25
4546	OD2	ASP	B	1256	-3.793	27.288	13.146	1	73.44
4547	N	GLU	B	1257	-3.333	31.379	16.66	1	70.16
4548	CA	GLU	B	1257	-3.959	32.355	17.535	1	69.38
4549	C	GLU	B	1257	-3.324	33.741	17.363	1	67.98
4550	O	GLU	B	1257	-4.021	34.736	17.168	1	66.91
4551	CB	GLU	B	1257	-3.854	31.9	18.989	1	71.08
4552	CG	GLU	B	1257	-4.666	32.752	19.943	1	79.31
4553	CD	GLU	B	1257	-4.33	32.504	21.401	1	83.72
4554	OE1	GLU	B	1257	-3.268	32.985	21.862	1	86.7
4555	OE2	GLU	B	1257	-5.133	31.841	22.088	1	86.01
4556	N	ALA	B	1258	-1.999	33.792	17.368	1	63.29
4557	CA	ALA	B	1258	-1.3	35.055	17.223	1	60.57
4558	C	ALA	B	1258	-1.461	35.663	15.844	1	61.7
4559	O	ALA	B	1258	-1.562	36.886	15.704	1	61.55
4560	CB	ALA	B	1258	0.153	34.869	17.525	1	60.8
4561	N	LYS	B	1259	-1.478	34.799	14.828	1	62.12
4562	CA	LYS	B	1259	-1.599	35.225	13.433	1	60.44
4563	C	LYS	B	1259	-2.955	35.851	13.166	1	61.2
4564	O	LYS	B	1259	-3.045	36.935	12.593	1	59.62
4565	CB	LYS	B	1259	-1.378	34.045	12.487	1	58.41
4566	CG	LYS	B	1259	-1.323	34.438	11.015	1	57.86
4567	CD	LYS	B	1259	-1.352	33.213	10.127	1	58.74
4568	CE	LYS	B	1259	-2.645	32.447	10.319	1	61.03
4569	NZ	LYS	B	1259	-2.675	31.156	9.596	1	63.9
4570	N	ASN	B	1260	-4.008	35.156	13.58	1	61.15
4571	CA	ASN	B	1260	-5.355	35.66	13.406	1	62.06
4572	C	ASN	B	1260	-5.492	37.005	14.129	1	61.36
4573	O	ASN	B	1260	-5.934	37.982	13.541	1	62.21
4574	CB	ASN	B	1260	-6.386	34.652	13.94	1	65.52
4575	CG	ASN	B	1260	-6.39	33.318	13.161	1	67.85
4576	OD1	ASN	B	1260	-6.67	32.257	13.728	1	69.36
4577	ND2	ASN	B	1260	-6.094	33.377	11.867	1	66.47
4578	N	TYR	B	1261	-5.049	37.075	15.38	1	61.18
4579	CA	TYR	B	1261	-5.154	38.315	16.14	1	59.38
4580	C	TYR	B	1261	-4.462	39.487	15.459	1	60.07
4581	O	TYR	B	1261	-5.082	40.513	15.223	1	62.69
4582	CB	TYR	B	1261	-4.618	38.156	17.568	1	54.17
4583	CG	TYR	B	1261	-4.846	39.396	18.386	1	50.61
4584	CD1	TYR	B	1261	-6.115	39.698	18.875	1	51.79
4585	CD2	TYR	B	1261	-3.826	40.323	18.583	1	51.69
4586	CE1	TYR	B	1261	-6.371	40.892	19.529	1	52.22
4587	CE2	TYR	B	1261	-4.062	41.536	19.235	1	53.13
4588	CZ	TYR	B	1261	-5.343	41.815	19.704	1	56.41
4589	OH	TYR	B	1261	-5.619	43.019	20.318	1	55.85
4590	N	MET	B	1262	-3.185	39.33	15.136	1	63.11
4591	CA	MET	B	1262	-2.417	40.392	14.486	1	65.26
4592	C	MET	B	1262	-2.973	40.799	13.108	1	68.67

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4593	O	MET	B	1262	-2.717	41.916	12.619	1	67.05
4594	CB	MET	B	1262	-0.962	39.949	14.352	1	64.37
4595	CG	MET	B	1262	-0.211	39.85	15.655	1	59.25
4596	SD	MET	B	1262	0.018	41.481	16.394	1	67.15
4597	CE	MET	B	1262	0.971	42.304	15.118	1	58.72
4598	N	LYS	B	1263	-3.713	39.875	12.491	1	72.15
4599	CA	LYS	B	1263	-4.33	40.067	11.174	1	75.66
4600	C	LYS	B	1263	-5.469	41.074	11.312	1	76.85
4601	O	LYS	B	1263	-5.491	42.096	10.632	1	77.11
4602	CB	LYS	B	1263	-4.903	38.732	10.675	1	76.85
4603	CG	LYS	B	1263	-4.698	38.397	9.199	1	79.3
4604	CD	LYS	B	1263	-3.306	37.827	8.928	1	79.93
4605	CE	LYS	B	1263	-3.221	37.108	7.576	1	81.06
4606	NZ	LYS	B	1263	-3.864	35.758	7.571	1	81.5
4607	N	GLY	B	1264	-6.397	40.777	12.219	1	78.8
4608	CA	GLY	B	1264	-7.539	41.646	12.452	1	81.83
4609	C	GLY	B	1264	-7.163	43.001	13.018	1	81.51
4610	O	GLY	B	1264	-7.882	43.98	12.869	1	81.91
4611	N	LEU	B	1265	-6.016	43.054	13.668	1	83.44
4612	CA	LEU	B	1265	-5.525	44.284	14.264	1	84.73
4613	C	LEU	B	1265	-5.23	45.323	13.186	1	85.19
4614	O	LEU	B	1265	-4.826	44.976	12.072	1	86.18
4615	CB	LEU	B	1265	-4.234	43.984	15.024	1	85.1
4616	CG	LEU	B	1265	-3.838	44.932	16.144	1	83.99
4617	CD1	LEU	B	1265	-4.807	44.721	17.284	1	84.37
4618	CD2	LEU	B	1265	-2.419	44.648	16.594	1	84.44
4619	N	PRO	B	1266	-5.47	46.612	13.486	1	86.14
4620	CA	PRO	B	1266	-5.215	47.709	12.539	1	85.42
4621	C	PRO	B	1266	-3.721	47.775	12.234	1	84.5
4622	O	PRO	B	1266	-2.945	46.96	12.723	1	86.42
4623	CB	PRO	B	1266	-5.644	48.945	13.329	1	85.91
4624	CG	PRO	B	1266	-6.754	48.42	14.199	1	88.17
4625	CD	PRO	B	1266	-6.193	47.102	14.677	1	87.57
4626	N	GLU	B	1267	-3.312	48.741	11.428	1	83.25
4627	CA	GLU	B	1267	-1.903	48.882	11.104	1	81.19
4628	C	GLU	B	1267	-1.411	50.118	11.848	1	79.24
4629	O	GLU	B	1267	-1.658	51.249	11.434	1	79.45
4630	CB	GLU	B	1267	-1.718	49.009	9.586	1	84.26
4631	CG	GLU	B	1267	-0.27	48.931	9.107	1	89.83
4632	CD	GLU	B	1267	-0.113	48.13	7.813	1	94.51
4633	OE1	GLU	B	1267	0.07	46.895	7.904	1	94.61
4634	OE2	GLU	B	1267	-0.164	48.73	6.71	1	95.62
4635	N	LEU	B	1268	-0.752	49.887	12.981	1	76.7
4636	CA	LEU	B	1268	-0.236	50.959	13.833	1	73.83
4637	C	LEU	B	1268	1.193	51.403	13.535	1	71.42
4638	O	LEU	B	1268	2.028	50.609	13.109	1	71.74
4639	CB	LEU	B	1268	-0.368	50.543	15.297	1	72.92
4640	CG	LEU	B	1268	-1.83	50.345	15.713	1	75.22
4641	CD1	LEU	B	1268	-1.97	49.261	16.769	1	75.1
4642	CD2	LEU	B	1268	-2.413	51.674	16.181	1	76.24
4643	N	GLU	B	1269	1.456	52.687	13.745	1	69.3
4644	CA	GLU	B	1269	2.778	53.253	13.51	1	68.33
4645	C	GLU	B	1269	3.51	53.472	14.84	1	68.25
4646	O	GLU	B	1269	2.887	53.727	15.871	1	66.89
4647	CB	GLU	B	1269	2.664	54.573	12.73	1	67.48
4648	N	LYS	B	1270	4.836	53.387	14.803	1	66.93

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4649	CA	LYS	B	1270	5.668	53.561	15.988	1	65.75
4650	C	LYS	B	1270	5.632	55.004	16.477	1	66.16
4651	O	LYS	B	1270	5.849	55.935	15.7	1	64.99
4652	CB	LYS	B	1270	7.11	53.152	15.666	1	66.19
4653	CG	LYS	B	1270	7.773	52.241	16.695	1	66.44
4654	CD	LYS	B	1270	8.293	52.985	17.917	1	67.33
4655	CE	LYS	B	1270	9.494	53.881	17.588	1	65.09
4656	NZ	LYS	B	1270	10.128	54.429	18.833	1	60.85
4657	N	LYS	B	1271	5.361	55.18	17.769	1	67.55
4658	CA	LYS	B	1271	5.303	56.508	18.383	1	67.77
4659	C	LYS	B	1271	6.647	56.811	19.017	1	67.69
4660	O	LYS	B	1271	7.36	55.897	19.424	1	67.47
4661	CB	LYS	B	1271	4.183	56.571	19.45	1	65.91
4662	N	ASP	B	1272	7.005	58.091	19.063	1	69.61
4663	CA	ASP	B	1272	8.263	58.513	19.664	1	69.98
4664	C	ASP	B	1272	8.058	58.314	21.153	1	69.48
4665	O	ASP	B	1272	7.026	58.714	21.682	1	70.79
4666	CB	ASP	B	1272	8.512	59.991	19.375	1	72.7
4667	CG	ASP	B	1272	9.923	60.425	19.713	1	74.97
4668	OD1	ASP	B	1272	10.25	60.564	20.918	1	75
4669	OD2	ASP	B	1272	10.706	60.632	18.759	1	78.18
4670	N	PHE	B	1273	9.024	57.697	21.829	1	68.18
4671	CA	PHE	B	1273	8.889	57.453	23.261	1	65.46
4672	C	PHE	B	1273	8.816	58.714	24.099	1	65.24
4673	O	PHE	B	1273	8.08	58.754	25.081	1	61.9
4674	CB	PHE	B	1273	9.983	56.513	23.774	1	64.16
4675	CG	PHE	B	1273	9.687	55.049	23.54	1	63.69
4676	CD1	PHE	B	1273	8.772	54.649	22.567	1	61.12
4677	CD2	PHE	B	1273	10.338	54.069	24.279	1	63.74
4678	CE1	PHE	B	1273	8.515	53.306	22.334	1	60.04
4679	CE2	PHE	B	1273	10.082	52.715	24.048	1	63.22
4680	CZ	PHE	B	1273	9.171	52.335	23.074	1	61.04
4681	N	ALA	B	1274	9.539	59.753	23.686	1	66.63
4682	CA	ALA	B	1274	9.542	61.025	24.408	1	69.62
4683	C	ALA	B	1274	8.14	61.632	24.491	1	70.5
4684	O	ALA	B	1274	7.856	62.443	25.377	1	69.92
4685	CB	ALA	B	1274	10.497	62.003	23.743	1	69.88
4686	N	SER	B	1275	7.275	61.217	23.563	1	72.43
4687	CA	SER	B	1275	5.884	61.673	23.487	1	73.84
4688	C	SER	B	1275	4.998	61.015	24.546	1	74.53
4689	O	SER	B	1275	3.901	61.491	24.82	1	75.39
4690	CB	SER	B	1275	5.319	61.388	22.096	1	71.41
4691	N	ILE	B	1276	5.48	59.914	25.118	1	77.16
4692	CA	ILE	B	1276	4.763	59.158	26.144	1	77.51
4693	C	ILE	B	1276	5.278	59.493	27.539	1	79
4694	O	ILE	B	1276	4.498	59.738	28.455	1	79.83
4695	CB	ILE	B	1276	4.956	57.642	25.949	1	77.77
4696	CG1	ILE	B	1276	4.703	57.255	24.496	1	76.62
4697	CG2	ILE	B	1276	4.026	56.864	26.868	1	77.73
4698	CD1	ILE	B	1276	5.015	55.809	24.212	1	79.55
4699	N	LEU	B	1277	6.597	59.452	27.7	1	80.74
4700	CA	LEU	B	1277	7.247	59.737	28.979	1	84.06
4701	C	LEU	B	1277	7.34	61.249	29.199	1	86.87
4702	O	LEU	B	1277	8.358	61.875	28.894	1	85.95
4703	CB	LEU	B	1277	8.64	59.106	28.995	1	82.05
4704	CG	LEU	B	1277	8.746	57.727	28.339	1	78.97

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4705	CD1	LEU	B	1277	10.171	57.254	28.36	1	76.91
4706	CD2	LEU	B	1277	7.835	56.744	29.036	1	79.91
4707	N	THR	B	1278	6.27	61.808	29.76	1	90.84
4708	CA	THR	B	1278	6.145	63.243	30.015	1	95.63
4709	C	THR	B	1278	7.367	63.958	30.606	1	97.4
4710	O	THR	B	1278	7.998	64.773	29.925	1	97.16
4711	CB	THR	B	1278	4.887	63.562	30.881	1	96.55
4712	OG1	THR	B	1278	4.847	62.699	32.027	1	97.43
4713	CG2	THR	B	1278	3.609	63.392	30.064	1	96.74
4714	N	ASN	B	1279	7.688	63.672	31.865	1	97.5
4715	CA	ASN	B	1279	8.816	64.331	32.521	1	97.54
4716	C	ASN	B	1279	10.112	63.507	32.643	1	95.91
4717	O	ASN	B	1279	10.955	63.765	33.515	1	96.48
4718	CB	ASN	B	1279	8.383	64.916	33.886	1	100
4719	CG	ASN	B	1279	7.771	63.865	34.852	1	100
4720	OD1	ASN	B	1279	7.607	64.136	36.051	1	99.54
4721	ND2	ASN	B	1279	7.423	62.685	34.33	1	100
4722	N	ALA	B	1280	10.284	62.544	31.74	1	92.84
4723	CA	ALA	B	1280	11.466	61.685	31.734	1	88.93
4724	C	ALA	B	1280	12.689	62.38	31.14	1	86.6
4725	O	ALA	B	1280	12.556	63.374	30.435	1	87.14
4726	CB	ALA	B	1280	11.173	60.409	30.972	1	88.35
4727	N	SER	B	1281	13.88	61.855	31.418	1	84.02
4728	CA	SER	B	1281	15.106	62.446	30.888	1	81.36
4729	C	SER	B	1281	15.379	61.907	29.475	1	80.26
4730	O	SER	B	1281	14.831	60.874	29.082	1	80.23
4731	CB	SER	B	1281	16.291	62.135	31.808	1	80.61
4732	OG	SER	B	1281	17.021	60.996	31.368	1	78.03
4733	N	PRO	B	1282	16.224	62.607	28.692	1	77.9
4734	CA	PRO	B	1282	16.578	62.212	27.325	1	75.18
4735	C	PRO	B	1282	17.242	60.834	27.247	1	73.25
4736	O	PRO	B	1282	16.805	59.972	26.472	1	72.63
4737	CB	PRO	B	1282	17.538	63.323	26.891	1	75.48
4738	CG	PRO	B	1282	18.127	63.809	28.174	1	75.62
4739	CD	PRO	B	1282	16.914	63.858	29.052	1	78.3
4740	N	LEU	B	1283	18.283	60.635	28.053	1	71.62
4741	CA	LEU	B	1283	19.02	59.364	28.104	1	68.65
4742	C	LEU	B	1283	18.113	58.211	28.547	1	67.58
4743	O	LEU	B	1283	18.264	57.07	28.084	1	66.85
4744	CB	LEU	B	1283	20.183	59.476	29.083	1	67.7
4745	CG	LEU	B	1283	21.339	60.392	28.714	1	67.35
4746	CD1	LEU	B	1283	22.242	60.618	29.916	1	66.53
4747	CD2	LEU	B	1283	22.1	59.773	27.563	1	65.79
4748	N	ALA	B	1284	17.199	58.519	29.471	1	64.43
4749	CA	ALA	B	1284	16.249	57.545	30.006	1	59.58
4750	C	ALA	B	1284	15.356	57.075	28.895	1	57.72
4751	O	ALA	B	1284	15.077	55.893	28.767	1	59.25
4752	CB	ALA	B	1284	15.408	58.18	31.106	1	61.25
4753	N	VAL	B	1285	14.904	58.025	28.087	1	56.46
4754	CA	VAL	B	1285	14.044	57.711	26.965	1	52.37
4755	C	VAL	B	1285	14.823	56.858	25.98	1	52.62
4756	O	VAL	B	1285	14.306	55.869	25.459	1	52.67
4757	CB	VAL	B	1285	13.535	58.993	26.294	1	46.38
4758	CG1	VAL	B	1285	12.781	58.673	25.043	1	46.24
4759	CG2	VAL	B	1285	12.64	59.722	27.236	1	45.78
4760	N	ASN	B	1286	16.089	57.204	25.769	1	53.19

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4761	CA	ASN	B	1286	16.882	56.434	24.828	1	55.25
4762	C	ASN	B	1286	17.013	54.992	25.302	1	53.6
4763	O	ASN	B	1286	16.718	54.077	24.546	1	53.58
4764	CB	ASN	B	1286	18.254	57.065	24.577	1	56.34
4765	CG	ASN	B	1286	19.043	56.31	23.519	1	58.72
4766	OD1	ASN	B	1286	18.835	56.494	22.317	1	61.07
4767	ND2	ASN	B	1286	19.914	55.416	23.962	1	58.48
4768	N	LEU	B	1287	17.401	54.796	26.56	1	52.93
4769	CA	LEU	B	1287	17.541	53.449	27.108	1	52.01
4770	C	LEU	B	1287	16.252	52.656	26.966	1	52.32
4771	O	LEU	B	1287	16.261	51.509	26.529	1	55.79
4772	CB	LEU	B	1287	17.928	53.497	28.582	1	49.29
4773	CG	LEU	B	1287	18.069	52.126	29.257	1	49.59
4774	CD1	LEU	B	1287	19.102	51.235	28.562	1	48.36
4775	CD2	LEU	B	1287	18.422	52.332	30.71	1	49.9
4776	N	LEU	B	1288	15.139	53.275	27.333	1	52.77
4777	CA	LEU	B	1288	13.839	52.625	27.238	1	52.03
4778	C	LEU	B	1288	13.568	52.187	25.807	1	53.2
4779	O	LEU	B	1288	13.146	51.055	25.557	1	50.69
4780	CB	LEU	B	1288	12.749	53.575	27.739	1	50.77
4781	CG	LEU	B	1288	12.651	53.597	29.265	1	47.67
4782	CD1	LEU	B	1288	11.625	54.601	29.738	1	49.99
4783	CD2	LEU	B	1288	12.267	52.206	29.737	1	49.57
4784	N	GLU	B	1289	13.873	53.085	24.873	1	56.08
4785	CA	GLU	B	1289	13.699	52.834	23.448	1	57.88
4786	C	GLU	B	1289	14.511	51.59	23.057	1	55.48
4787	O	GLU	B	1289	14.044	50.752	22.284	1	57.31
4788	CB	GLU	B	1289	14.158	54.062	22.651	1	60.3
4789	CG	GLU	B	1289	13.409	54.308	21.35	1	69.07
4790	CD	GLU	B	1289	12.532	55.562	21.39	1	75.71
4791	OE1	GLU	B	1289	13.025	56.647	21.781	1	77.13
4792	OE2	GLU	B	1289	11.345	55.467	21.005	1	78.96
4793	N	LYS	B	1290	15.701	51.455	23.63	1	53.91
4794	CA	LYS	B	1290	16.572	50.313	23.354	1	56.54
4795	C	LYS	B	1290	16.103	49.029	24.043	1	55
4796	O	LYS	B	1290	16.398	47.931	23.567	1	56.1
4797	CB	LYS	B	1290	18.012	50.615	23.774	1	59.63
4798	CG	LYS	B	1290	18.82	51.418	22.768	1	65.47
4799	CD	LYS	B	1290	20.177	51.801	23.344	1	68.89
4800	CE	LYS	B	1290	21.126	52.353	22.284	1	70.03
4801	NZ	LYS	B	1290	20.585	53.559	21.593	1	76.91
4802	N	MET	B	1291	15.417	49.165	25.18	1	51.73
4803	CA	MET	B	1291	14.913	47.995	25.907	1	52.36
4804	C	MET	B	1291	13.555	47.521	25.385	1	51.34
4805	O	MET	B	1291	13.272	46.327	25.372	1	47.34
4806	CB	MET	B	1291	14.802	48.255	27.416	1	50.01
4807	CG	MET	B	1291	16.095	48.612	28.097	1	50.51
4808	SD	MET	B	1291	15.987	48.458	29.879	1	54.34
4809	CE	MET	B	1291	15.499	50.088	30.376	1	48.91
4810	N	LEU	B	1292	12.729	48.454	24.928	1	52.59
4811	CA	LEU	B	1292	11.406	48.096	24.437	1	51.71
4812	C	LEU	B	1292	11.237	47.921	22.936	1	51.8
4813	O	LEU	B	1292	10.163	48.152	22.388	1	53.68
4814	CB	LEU	B	1292	10.381	49.073	24.996	1	49.81
4815	CG	LEU	B	1292	10.265	48.902	26.507	1	43.92
4816	CD1	LEU	B	1292	9.328	49.934	27.07	1	46.13

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4817	CD2	LEU	B	1292	9.758	47.485	26.802	1	44.69
4818	N	VAL	B	1293	12.3	47.506	22.268	1	55.13
4819	CA	VAL	B	1293	12.246	47.27	20.833	1	55.88
4820	C	VAL	B	1293	11.467	45.981	20.636	1	57
4821	O	VAL	B	1293	11.569	45.059	21.438	1	58.7
4822	CB	VAL	B	1293	13.646	47.169	20.231	1	55.38
4823	CG1	VAL	B	1293	13.602	46.431	18.91	1	58.99
4824	CG2	VAL	B	1293	14.212	48.584	20.023	1	57.62
4825	N	LEU	B	1294	10.659	45.948	19.586	1	58.16
4826	CA	LEU	B	1294	9.8	44.816	19.281	1	57.29
4827	C	LEU	B	1294	10.57	43.563	18.867	1	58.55
4828	O	LEU	B	1294	10.149	42.429	19.124	1	56.4
4829	CB	LEU	B	1294	8.829	45.249	18.183	1	56.93
4830	CG	LEU	B	1294	7.611	44.35	18.02	1	61.81
4831	CD1	LEU	B	1294	6.749	44.437	19.261	1	61.22
4832	CD2	LEU	B	1294	6.837	44.756	16.796	1	62.66
4833	N	ASP	B	1295	11.704	43.808	18.22	1	63.7
4834	CA	ASP	B	1295	12.619	42.797	17.697	1	66.56
4835	C	ASP	B	1295	13.536	42.308	18.815	1	66.13
4836	O	ASP	B	1295	14.537	42.951	19.136	1	66.23
4837	CB	ASP	B	1295	13.448	43.434	16.561	1	70.74
4838	CG	ASP	B	1295	14.362	42.437	15.839	1	76.92
4839	OD1	ASP	B	1295	14.219	41.198	16.033	1	77.65
4840	OD2	ASP	B	1295	15.225	42.916	15.056	1	75.82
4841	N	ALA	B	1296	13.194	41.16	19.388	1	64.53
4842	CA	ALA	B	1296	13.966	40.569	20.471	1	65.27
4843	C	ALA	B	1296	15.479	40.597	20.257	1	67.51
4844	O	ALA	B	1296	16.221	40.839	21.202	1	71.04
4845	CB	ALA	B	1296	13.506	39.145	20.708	1	66.62
4846	N	GLU	B	1297	15.934	40.371	19.025	1	68.4
4847	CA	GLU	B	1297	17.368	40.359	18.721	1	69.59
4848	C	GLU	B	1297	18.103	41.69	18.87	1	68.8
4849	O	GLU	B	1297	19.209	41.72	19.398	1	67.73
4850	CB	GLU	B	1297	17.614	39.789	17.322	1	73.1
4851	CG	GLU	B	1297	17.217	38.324	17.16	1	76.58
4852	CD	GLU	B	1297	18.095	37.366	17.959	1	76.43
4853	OE1	GLU	B	1297	19.337	37.418	17.794	1	75.95
4854	OE2	GLU	B	1297	17.538	36.546	18.727	1	71.42
4855	N	GLN	B	1298	17.505	42.775	18.379	1	70.63
4856	CA	GLN	B	1298	18.113	44.116	18.461	1	72.42
4857	C	GLN	B	1298	17.933	44.715	19.854	1	70.29
4858	O	GLN	B	1298	18.52	45.757	20.182	1	70.45
4859	CB	GLN	B	1298	17.48	45.075	17.433	1	79.12
4860	CG	GLN	B	1298	17.606	44.655	15.964	1	85.31
4861	CD	GLN	B	1298	19.047	44.532	15.513	1	89.05
4862	OE1	GLN	B	1298	19.427	43.561	14.839	1	87.96
4863	NE2	GLN	B	1298	19.867	45.514	15.895	1	90.97
4864	N	ARG	B	1299	17.105	44.053	20.66	1	66.4
4865	CA	ARG	B	1299	16.818	44.499	22.014	1	62.11
4866	C	ARG	B	1299	18.079	44.4	22.862	1	61.11
4867	O	ARG	B	1299	18.751	43.361	22.891	1	61.27
4868	CB	ARG	B	1299	15.68	43.659	22.608	1	59.93
4869	CG	ARG	B	1299	14.971	44.296	23.803	1	55.45
4870	CD	ARG	B	1299	13.464	44.128	23.676	1	52.46
4871	NE	ARG	B	1299	13.026	42.783	23.992	1	49.75
4872	CZ	ARG	B	1299	11.996	42.161	23.421	1	45.3

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4873	NH1	ARG	B	1299	11.271	42.735	22.485	1	37.8
4874	NH2	ARG	B	1299	11.696	40.946	23.803	1	43.43
4875	N	VAL	B	1300	18.398	45.499	23.536	1	60.09
4876	CA	VAL	B	1300	19.58	45.586	24.386	1	58.37
4877	C	VAL	B	1300	19.643	44.438	25.406	1	58.5
4878	O	VAL	B	1300	18.621	43.846	25.757	1	59.18
4879	CB	VAL	B	1300	19.605	46.968	25.107	1	56.62
4880	CG1	VAL	B	1300	19.034	46.87	26.499	1	54.15
4881	CG2	VAL	B	1300	20.993	47.551	25.108	1	53.94
4882	N	THR	B	1301	20.85	44.067	25.815	1	59.53
4883	CA	THR	B	1301	21.01	43.014	26.818	1	58.64
4884	C	THR	B	1301	21.31	43.714	28.126	1	58.82
4885	O	THR	B	1301	21.614	44.91	28.139	1	57.1
4886	CB	THR	B	1301	22.189	42.052	26.521	1	57.11
4887	OG1	THR	B	1301	23.422	42.782	26.547	1	55.86
4888	CG2	THR	B	1301	22.005	41.354	25.178	1	49.79
4889	N	ALA	B	1302	21.24	42.96	29.219	1	58.97
4890	CA	ALA	B	1302	21.511	43.505	30.539	1	57.86
4891	C	ALA	B	1302	22.907	44.107	30.567	1	56.43
4892	O	ALA	B	1302	23.107	45.202	31.101	1	55.91
4893	CB	ALA	B	1302	21.373	42.424	31.581	1	58.03
4894	N	GLY	B	1303	23.859	43.391	29.966	1	57.56
4895	CA	GLY	B	1303	25.227	43.876	29.903	1	59.47
4896	C	GLY	B	1303	25.273	45.219	29.187	1	60.75
4897	O	GLY	B	1303	25.758	46.226	29.735	1	60.75
4898	N	GLU	B	1304	24.715	45.234	27.975	1	59.98
4899	CA	GLU	B	1304	24.659	46.435	27.148	1	60.78
4900	C	GLU	B	1304	23.889	47.531	27.873	1	58.84
4901	O	GLU	B	1304	24.313	48.686	27.896	1	60.91
4902	CB	GLU	B	1304	23.983	46.143	25.807	1	63.53
4903	CG	GLU	B	1304	24.674	45.123	24.904	1	67.68
4904	CD	GLU	B	1304	23.878	44.845	23.621	1	74.21
4905	OE1	GLU	B	1304	23.297	45.802	23.05	1	78.48
4906	OE2	GLU	B	1304	23.831	43.674	23.177	1	74.31
4907	N	ALA	B	1305	22.773	47.147	28.486	1	56.09
4908	CA	ALA	B	1305	21.921	48.063	29.231	1	53.83
4909	C	ALA	B	1305	22.731	48.843	30.253	1	54.47
4910	O	ALA	B	1305	22.653	50.072	30.317	1	55.75
4911	CB	ALA	B	1305	20.822	47.292	29.924	1	51.36
4912	N	LEU	B	1306	23.529	48.123	31.033	1	54.84
4913	CA	LEU	B	1306	24.37	48.724	32.065	1	55.91
4914	C	LEU	B	1306	25.407	49.67	31.476	1	59.33
4915	O	LEU	B	1306	25.729	50.704	32.068	1	61.01
4916	CB	LEU	B	1306	25.084	47.621	32.833	1	53
4917	CG	LEU	B	1306	24.24	46.747	33.754	1	47.56
4918	CD1	LEU	B	1306	25.057	45.571	34.216	1	43.12
4919	CD2	LEU	B	1306	23.776	47.565	34.943	1	48.23
4920	N	ALA	B	1307	25.927	49.297	30.307	1	63.38
4921	CA	ALA	B	1307	26.931	50.088	29.584	1	64.24
4922	C	ALA	B	1307	26.412	51.429	29.027	1	63.84
4923	O	ALA	B	1307	27.211	52.28	28.623	1	66.62
4924	CB	ALA	B	1307	27.526	49.257	28.454	1	59.56
4925	N	HIS	B	1308	25.092	51.624	29.048	1	59.56
4926	CA	HIS	B	1308	24.463	52.835	28.529	1	56.83
4927	C	HIS	B	1308	24.811	54.127	29.284	1	58.09
4928	O	HIS	B	1308	25.02	54.121	30.493	1	61.2

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4929	CB	HIS	B	1308	22.956	52.629	28.496	1	51.82
4930	CG	HIS	B	1308	22.22	53.628	27.662	1	46.18
4931	ND1	HIS	B	1308	21.771	54.831	28.166	1	47.87
4932	CD2	HIS	B	1308	21.809	53.58	26.373	1	37.9
4933	CE1	HIS	B	1308	21.107	55.478	27.225	1	43.09
4934	NE2	HIS	B	1308	21.114	54.74	26.129	1	40.01
4935	N	PRO	B	1309	24.883	55.256	28.569	1	59.7
4936	CA	PRO	B	1309	25.204	56.551	29.174	1	62.3
4937	C	PRO	B	1309	24.259	56.996	30.293	1	63.3
4938	O	PRO	B	1309	24.533	57.997	30.974	1	64.91
4939	CB	PRO	B	1309	25.121	57.506	27.983	1	63.19
4940	CG	PRO	B	1309	25.583	56.652	26.85	1	62.09
4941	CD	PRO	B	1309	24.82	55.377	27.102	1	61.18
4942	N	TYR	B	1310	23.134	56.294	30.45	1	61.17
4943	CA	TYR	B	1310	22.159	56.628	31.493	1	61.55
4944	C	TYR	B	1310	22.755	56.314	32.864	1	61.07
4945	O	TYR	B	1310	22.593	57.071	33.826	1	57.44
4946	CB	TYR	B	1310	20.858	55.826	31.288	1	59.61
4947	CG	TYR	B	1310	19.801	56.056	32.356	1	59.47
4948	CD1	TYR	B	1310	19.282	57.337	32.593	1	58.59
4949	CD2	TYR	B	1310	19.316	54.994	33.134	1	58.93
4950	CE1	TYR	B	1310	18.308	57.558	33.568	1	56.43
4951	CE2	TYR	B	1310	18.335	55.205	34.121	1	58.02
4952	CZ	TYR	B	1310	17.836	56.496	34.325	1	57.9
4953	OH	TYR	B	1310	16.855	56.74	35.261	1	55.83
4954	N	PHE	B	1311	23.487	55.207	32.907	1	63.08
4955	CA	PHE	B	1311	24.122	54.708	34.118	1	68.47
4956	C	PHE	B	1311	25.569	55.196	34.253	1	72.32
4957	O	PHE	B	1311	26.386	54.571	34.935	1	73.06
4958	CB	PHE	B	1311	24.077	53.169	34.112	1	64.71
4959	CG	PHE	B	1311	22.681	52.593	33.984	1	59.83
4960	CD1	PHE	B	1311	21.689	52.918	34.9	1	58.99
4961	CD2	PHE	B	1311	22.364	51.739	32.941	1	58.65
4962	CE1	PHE	B	1311	20.408	52.4	34.77	1	59.47
4963	CE2	PHE	B	1311	21.079	51.218	32.809	1	57.68
4964	CZ	PHE	B	1311	20.104	51.547	33.719	1	54.46
4965	N	GLU	B	1312	25.856	56.339	33.634	1	76.5
4966	CA	GLU	B	1312	27.19	56.949	33.632	1	78.82
4967	C	GLU	B	1312	27.778	57.181	35.025	1	75.94
4968	O	GLU	B	1312	28.882	56.731	35.313	1	75.3
4969	CB	GLU	B	1312	27.141	58.278	32.855	1	85.41
4970	CG	GLU	B	1312	28.489	58.984	32.646	1	89.87
4971	CD	GLU	B	1312	28.337	60.388	32.051	1	93.07
4972	OE1	GLU	B	1312	27.635	61.234	32.66	1	95.02
4973	OE2	GLU	B	1312	28.931	60.649	30.978	1	94.03
4974	N	SER	B	1313	27.024	57.865	35.879	1	73.48
4975	CA	SER	B	1313	27.465	58.175	37.231	1	73.98
4976	C	SER	B	1313	27.536	56.974	38.174	1	73.7
4977	O	SER	B	1313	27.809	57.13	39.366	1	73.28
4978	CB	SER	B	1313	26.566	59.255	37.847	1	73.88
4979	OG	SER	B	1313	25.26	58.767	38.084	1	72.13
4980	N	LEU	B	1314	27.319	55.778	37.645	1	73.19
4981	CA	LEU	B	1314	27.349	54.587	38.48	1	75.67
4982	C	LEU	B	1314	28.277	53.491	37.948	1	78.49
4983	O	LEU	B	1314	28.727	52.636	38.714	1	78.97
4984	CB	LEU	B	1314	25.927	54.029	38.649	1	74.26

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
4985	CG	LEU	B	1314	24.789	54.937	39.148	1	71.09
4986	CD1	LEU	B	1314	23.467	54.208	39.035	1	69.07
4987	CD2	LEU	B	1314	25.023	55.378	40.575	1	69.89
4988	N	HIS	B	1315	28.584	53.548	36.649	1	81.55
4989	CA	HIS	B	1315	29.439	52.566	35.954	1	83.48
4990	C	HIS	B	1315	30.811	52.231	36.586	1	84.56
4991	O	HIS	B	1315	31.324	53.047	37.389	1	84.58
4992	CB	HIS	B	1315	29.614	52.982	34.475	1	81.89
4993	OXT	HIS	B	1315	31.364	51.146	36.262	1	83.36
4994	N	GLN	B	1322	33.191	37.322	36.761	1	90.82
4995	CA	GLN	B	1322	32.735	36.168	35.923	1	92.08
4996	C	GLN	B	1322	31.847	35.232	36.756	1	92.21
4997	O	GLN	B	1322	32.034	35.123	37.983	1	91.78
4998	CB	GLN	B	1322	33.94	35.411	35.358	1	93.05
4999	N	VAL	B	1323	30.899	34.552	36.095	1	88.96
5000	CA	VAL	B	1323	29.961	33.665	36.799	1	86.14
5001	C	VAL	B	1323	29.865	32.199	36.37	1	84.66
5002	O	VAL	B	1323	30.009	31.846	35.192	1	81.99
5003	CB	VAL	B	1323	28.518	34.243	36.817	1	83.7
5004	CG1	VAL	B	1323	28.536	35.737	37.113	1	81.83
5005	CG2	VAL	B	1323	27.823	33.958	35.518	1	81.75
5006	N	GLN	B	1324	29.532	31.37	37.356	1	83.53
5007	CA	GLN	B	1324	29.385	29.931	37.181	1	83.72
5008	C	GLN	B	1324	27.998	29.582	36.675	1	81.62
5009	O	GLN	B	1324	27.004	29.778	37.378	1	78.62
5010	CB	GLN	B	1324	29.655	29.202	38.512	1	84.79
5011	N	LYS	B	1325	27.944	29.042	35.462	1	80.82
5012	CA	LYS	B	1325	26.677	28.653	34.861	1	80.84
5013	C	LYS	B	1325	25.979	27.572	35.674	1	80.58
5014	O	LYS	B	1325	26.62	26.65	36.176	1	83.59
5015	CB	LYS	B	1325	26.882	28.177	33.419	1	79.07
5016	CG	LYS	B	1325	27.298	29.284	32.451	1	79.16
5017	CD	LYS	B	1325	26.965	28.902	31.021	1	78.85
5018	CE	LYS	B	1325	25.514	28.446	30.922	1	78.35
5019	NZ	LYS	B	1325	25.086	28.186	29.521	1	82.1
5020	N	TYR	B	1326	24.674	27.729	35.858	1	79.6
5021	CA	TYR	B	1326	23.875	26.758	36.595	1	80.04
5022	C	TYR	B	1326	23.767	25.487	35.733	1	83.83
5023	O	TYR	B	1326	23.733	25.566	34.51	1	84.12
5024	CB	TYR	B	1326	22.503	27.365	36.888	1	74.1
5025	CG	TYR	B	1326	21.487	26.414	37.458	1	69.26
5026	CD1	TYR	B	1326	21.497	26.071	38.803	1	69.12
5027	CD2	TYR	B	1326	20.505	25.859	36.648	1	69.77
5028	CE1	TYR	B	1326	20.547	25.193	39.328	1	69.52
5029	CE2	TYR	B	1326	19.555	24.983	37.158	1	70.51
5030	CZ	TYR	B	1326	19.579	24.653	38.495	1	69.18
5031	OH	TYR	B	1326	18.632	23.778	38.979	1	71.04
5032	N	ASP	B	1327	23.743	24.32	36.37	1	88.48
5033	CA	ASP	B	1327	23.666	23.045	35.652	1	93.54
5034	C	ASP	B	1327	22.555	22.174	36.255	1	95.72
5035	O	ASP	B	1327	22.144	22.427	37.384	1	99.03
5036	CB	ASP	B	1327	25.02	22.339	35.782	1	96.66
5037	CG	ASP	B	1327	25.209	21.237	34.763	1	100
5038	OD1	ASP	B	1327	25.101	21.532	33.541	1	99.85
5039	OD2	ASP	B	1327	25.476	20.085	35.194	1	100
5040	N	ASP	B	1328	22.078	21.151	35.538	1	97.29

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
5041	CA	ASP	B	1328	21.011	20.297	36.091	1	99.52
5042	C	ASP	B	1328	20.601	19.033	35.302	1	100
5043	O	ASP	B	1328	21.098	18.754	34.202	1	100
5044	CB	ASP	B	1328	19.756	21.159	36.369	1	100
5045	CG	ASP	B	1328	18.714	20.449	37.238	1	100
5046	OD1	ASP	B	1328	19.012	20.156	38.417	1	98.29
5047	OD2	ASP	B	1328	17.596	20.184	36.732	1	100
5048	N	SER	B	1329	19.709	18.263	35.934	1	100
5049	CA	SER	B	1329	19.116	17.033	35.405	1	99.65
5050	C	SER	B	1329	17.759	16.801	36.127	1	99.45
5051	O	SER	B	1329	17.721	16.19	37.218	1	98.29
5052	CB	SER	B	1329	20.074	15.831	35.571	1	97.33
5053	OG	SER	B	1329	20.4	15.573	36.927	1	93.65
5054	OXT	SER	B	1329	16.732	17.304	35.617	1	98.81
5055	N	ARG	B	1335	9.439	13.254	34.69	1	95.6
5056	CA	ARG	B	1335	9.514	12.74	36.088	1	96.62
5057	C	ARG	B	1335	8.129	12.68	36.737	1	97.23
5058	O	ARG	B	1335	7.254	13.488	36.417	1	96.98
5059	CB	ARG	B	1335	10.457	13.618	36.918	1	96.54
5060	N	THR	B	1336	7.936	11.716	37.641	1	98.37
5061	CA	THR	B	1336	6.656	11.537	38.35	1	99.77
5062	C	THR	B	1336	6.471	12.546	39.496	1	99.59
5063	O	THR	B	1336	7.422	13.227	39.882	1	100
5064	CB	THR	B	1336	6.501	10.079	38.92	1	100
5065	OG1	THR	B	1336	7.503	9.824	39.912	1	98.6
5066	CG2	THR	B	1336	6.634	9.038	37.808	1	100
5067	N	LEU	B	1337	5.249	12.652	40.024	1	98.78
5068	CA	LEU	B	1337	4.969	13.572	41.129	1	99.13
5069	C	LEU	B	1337	5.873	13.21	42.305	1	100
5070	O	LEU	B	1337	6.419	14.088	42.98	1	100
5071	CB	LEU	B	1337	3.496	13.495	41.544	1	97.48
5072	N	ASP	B	1338	6.063	11.908	42.508	1	100
5073	CA	ASP	B	1338	6.913	11.406	43.581	1	100
5074	C	ASP	B	1338	8.407	11.557	43.303	1	100
5075	O	ASP	B	1338	9.218	11.46	44.228	1	100
5076	CB	ASP	B	1338	6.574	9.951	43.899	1	100
5077	CG	ASP	B	1338	5.329	9.821	44.747	1	100
5078	OD1	ASP	B	1338	4.407	10.659	44.592	1	100
5079	OD2	ASP	B	1338	5.284	8.886	45.578	1	100
5080	N	GLU	B	1339	8.772	11.755	42.035	1	99.94
5081	CA	GLU	B	1339	10.175	11.954	41.666	1	99.4
5082	C	GLU	B	1339	10.56	13.395	41.989	1	98.48
5083	O	GLU	B	1339	11.644	13.653	42.516	1	99.33
5084	CB	GLU	B	1339	10.416	11.645	40.182	1	99.75
5085	CG	GLU	B	1339	10.657	10.158	39.893	1	100
5086	CD	GLU	B	1339	10.823	9.844	38.409	1	100
5087	OE1	GLU	B	1339	11.768	10.374	37.783	1	99.61
5088	OE2	GLU	B	1339	10.014	9.054	37.873	1	100
5089	N	TRP	B	1340	9.651	14.324	41.697	1	96.8
5090	CA	TRP	B	1340	9.871	15.739	41.978	1	94.77
5091	C	TRP	B	1340	9.93	15.935	43.487	1	94.28
5092	O	TRP	B	1340	10.818	16.611	44.003	1	94.83
5093	CB	TRP	B	1340	8.738	16.594	41.398	1	91.56
5094	CG	TRP	B	1340	8.822	16.805	39.923	1	87.42
5095	CD1	TRP	B	1340	7.96	16.335	38.983	1	86.35
5096	CD2	TRP	B	1340	9.828	17.541	39.214	1	85.91

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
5097	NE1	TRP	B	1340	8.364	16.728	37.73	1	85.95
5098	CE2	TRP	B	1340	9.509	17.47	37.844	1	84.93
5099	CE3	TRP	B	1340	10.972	18.251	39.607	1	85.21
5100	CZ2	TRP	B	1340	10.291	18.083	36.856	1	83.82
5101	CZ3	TRP	B	1340	11.751	18.86	38.622	1	84.21
5102	CH2	TRP	B	1340	11.404	18.77	37.263	1	82.56
5103	N	LYS	B	1341	8.979	15.316	44.179	1	93.1
5104	CA	LYS	B	1341	8.87	15.378	45.633	1	91.46
5105	C	LYS	B	1341	10.155	14.868	46.29	1	90.23
5106	O	LYS	B	1341	10.673	15.49	47.22	1	89.13
5107	CB	LYS	B	1341	7.666	14.536	46.063	1	91.94
5108	CG	LYS	B	1341	7.238	14.636	47.513	1	92.72
5109	CD	LYS	B	1341	5.889	13.929	47.68	1	95.18
5110	CE	LYS	B	1341	5.456	13.808	49.135	1	96.47
5111	NZ	LYS	B	1341	4.096	13.201	49.263	1	95.26
5112	N	ARG	B	1342	10.687	13.767	45.76	1	90.08
5113	CA	ARG	B	1342	11.915	13.156	46.272	1	89.34
5114	C	ARG	B	1342	13.148	13.988	45.925	1	87.69
5115	O	ARG	B	1342	13.983	14.255	46.795	1	88.78
5116	CB	ARG	B	1342	12.072	11.721	45.738	1	89.2
5117	N	VAL	B	1343	13.266	14.38	44.656	1	84.09
5118	CA	VAL	B	1343	14.393	15.189	44.203	1	82.03
5119	C	VAL	B	1343	14.44	16.494	45.012	1	82.27
5120	O	VAL	B	1343	15.516	16.973	45.378	1	82.21
5121	CB	VAL	B	1343	14.264	15.485	42.71	1	79.36
5122	N	THR	B	1344	13.259	17.03	45.325	1	80.68
5123	CA	THR	B	1344	13.123	18.265	46.093	1	78.06
5124	C	THR	B	1344	13.556	18.059	47.538	1	77.6
5125	O	THR	B	1344	14.425	18.784	48.038	1	76.34
5126	CB	THR	B	1344	11.663	18.788	46.06	1	75.74
5127	OG1	THR	B	1344	11.321	19.15	44.72	1	74.27
5128	CG2	THR	B	1344	11.495	20	46.954	1	74.75
5129	N	TYR	B	1345	12.952	17.064	48.191	1	77
5130	CA	TYR	B	1345	13.249	16.731	49.587	1	76.12
5131	C	TYR	B	1345	14.75	16.655	49.815	1	74.18
5132	O	TYR	B	1345	15.251	17.135	50.826	1	74.4
5133	CB	TYR	B	1345	12.598	15.396	49.96	1	78.36
5134	CG	TYR	B	1345	12.65	15.062	51.434	1	80.34
5135	CD1	TYR	B	1345	12.062	15.902	52.379	1	81.68
5136	CD2	TYR	B	1345	13.29	13.905	51.888	1	80.51
5137	CE1	TYR	B	1345	12.111	15.602	53.744	1	83.58
5138	CE2	TYR	B	1345	13.345	13.596	53.25	1	80.89
5139	CZ	TYR	B	1345	12.756	14.449	54.171	1	83.44
5140	OH	TYR	B	1345	12.828	14.173	55.523	1	86.8
5141	N	LYS	B	1346	15.459	16.079	48.848	1	73.97
5142	CA	LYS	B	1346	16.911	15.946	48.91	1	74.77
5143	C	LYS	B	1346	17.6	17.321	48.909	1	75.13
5144	O	LYS	B	1346	18.493	17.577	49.721	1	75.76
5145	CB	LYS	B	1346	17.415	15.078	47.744	1	72.36
5146	N	GLU	B	1347	17.159	18.213	48.021	1	75.84
5147	CA	GLU	B	1347	17.735	19.554	47.933	1	74.51
5148	C	GLU	B	1347	17.389	20.398	49.158	1	73.98
5149	O	GLU	B	1347	18.054	21.397	49.434	1	74.18
5150	CB	GLU	B	1347	17.285	20.262	46.647	1	72.61
5151	CG	GLU	B	1347	17.941	19.744	45.353	1	73.15
5152	CD	GLU	B	1347	19.427	20.115	45.208	1	76.28

Figure 1

Atom	Atom Type	Residue		#	X	Y	Z	OCC	B
5153	OE1	GLU	B	1347	19.819	21.264	45.541	1	74.83
5154	OE2	GLU	B	1347	20.205	19.257	44.728	1	76.09
5155	N	VAL	B	1348	16.355	19.993	49.892	1	73.02
5156	CA	VAL	B	1348	15.95	20.723	51.091	1	73.71
5157	C	VAL	B	1348	16.856	20.339	52.261	1	75.29
5158	O	VAL	B	1348	17.356	21.203	52.991	1	75.92
5159	CB	VAL	B	1348	14.472	20.438	51.483	1	72.39
5160	CG1	VAL	B	1348	14.107	21.195	52.742	1	70.67
5161	CG2	VAL	B	1348	13.529	20.85	50.368	1	72.79
5162	N	LEU	B	1349	17.089	19.039	52.413	1	75.21
5163	CA	LEU	B	1349	17.923	18.534	53.499	1	73.36
5164	C	LEU	B	1349	19.406	18.823	53.318	1	71.93
5165	O	LEU	B	1349	20.148	18.903	54.301	1	72.07
5166	CB	LEU	B	1349	17.7	17.032	53.682	1	73.5
5167	CG	LEU	B	1349	16.258	16.621	54.005	1	76.3
5168	CD1	LEU	B	1349	16.22	15.128	54.292	1	75.07
5169	CD2	LEU	B	1349	15.709	17.419	55.203	1	74.88
5170	N	SER	B	1350	19.835	18.987	52.069	1	69.7
5171	CA	SER	B	1350	21.241	19.257	51.775	1	69.38
5172	C	SER	B	1350	21.628	20.733	51.914	1	69.94
5173	O	SER	B	1350	22.752	21.125	51.583	1	68.66
5174	CB	SER	B	1350	21.617	18.731	50.374	1	69.35
5175	OG	SER	B	1350	20.938	19.402	49.322	1	68.19
5176	N	PHE	B	1351	20.718	21.543	52.444	1	68.17
5177	CA	PHE	B	1351	21.006	22.955	52.584	1	69.97
5178	C	PHE	B	1351	21.881	23.323	53.769	1	71.08
5179	O	PHE	B	1351	21.565	22.995	54.909	1	72.12
5180	CB	PHE	B	1351	19.719	23.758	52.664	1	69.27
5181	CG	PHE	B	1351	19.941	25.246	52.675	1	67.44
5182	CD1	PHE	B	1351	20.399	25.902	51.535	1	68.6
5183	CD2	PHE	B	1351	19.72	25.984	53.826	1	65.72
5184	CE1	PHE	B	1351	20.634	27.269	51.552	1	67.31
5185	CE2	PHE	B	1351	19.951	27.347	53.85	1	64.46
5186	CZ	PHE	B	1351	20.409	27.989	52.713	1	65
5187	N	LYS	B	1352	22.956	24.05	53.489	1	70.89
5188	CA	LYS	B	1352	23.865	24.51	54.528	1	71.5
5189	C	LYS	B	1352	23.766	26.034	54.543	1	71.96
5190	O	LYS	B	1352	23.996	26.683	53.53	1	72.27
5191	CB	LYS	B	1352	25.288	24.066	54.219	1	71.53
5192	N	PRO	B	1353	23.386	26.617	55.686	1	73.32
5193	CA	PRO	B	1353	23.228	28.063	55.909	1	76.72
5194	C	PRO	B	1353	24.407	28.968	55.496	1	78.51
5195	O	PRO	B	1353	25.456	28.441	55.057	1	79.15
5196	CB	PRO	B	1353	22.962	28.14	57.413	1	76.75
5197	CG	PRO	B	1353	22.188	26.884	57.666	1	76.61
5198	CD	PRO	B	1353	22.983	25.859	56.883	1	75.53
5199	OXT	PRO	B	1353	24.258	30.21	55.615	1	78.87
5200		PRO	B	1353					
5201	MG		MG		401	41.849	77.432	8.11	1
5202	MG		MG		402	47.016	76.86	9.61	1
5203	MG		MG		1401	5.69	38.173	43.7	1
5204	MG		MG		1402	6.189	32.966	42.1	1
5205	PG	ANP		400	44.037	79.054	8.861	1	66.71
5206	O1G	ANP		400	43.871	80.603	8.797	1	65.28
5207	O2G	ANP		400	42.804	78.446	9.688	1	64.26
5208	O3G	ANP		400	45.415	78.794	9.622	1	61.75

Figure 1

Atom	Atom Type	Residue	#	X	Y	Z	OCC	B
5209	PB	ANP	400	45.207	78.285	6.471	1	53.03
5210	O1B	ANP	400	45.357	79.52	5.523	1	54.98
5211	O2B	ANP	400	46.444	77.845	7.274	1	44.5
5212	N3B	ANP	400	44.026	78.547	7.417	1	55.71
5213	PA	ANP	400	43.636	76.122	5.359	1	45.13
5214	O1A	ANP	400	44.218	74.72	4.957	1	43.29
5215	O2A	ANP	400	42.982	76.037	6.707	1	39.7
5216	O3A	ANP	400	44.879	77.226	5.333	1	46.4
5217	O5*	ANP	400	42.52	76.556	4.302	1	44.29
5218	C5*	ANP	400	41.83	77.858	4.367	1	40.83
5219	C4*	ANP	400	40.642	77.72	3.427	1	40.7
5220	O4*	ANP	400	41.036	76.944	2.298	1	42.85
5221	C3*	ANP	400	39.56	76.822	4.049	1	44.36
5222	O3*	ANP	400	38.609	77.63	4.745	1	50.96
5223	C2*	ANP	400	38.862	76.098	2.89	1	40.35
5224	O2*	ANP	400	37.997	76.921	2.171	1	43.36
5225	C1*	ANP	400	40.071	75.951	1.995	1	37.7
5226	N9	ANP	400	40.475	74.651	1.773	1	38.51
5227	C8	ANP	400	41.646	74.092	2.267	1	41.44
5228	N7	ANP	400	41.838	72.823	1.829	1	36.45
5229	C5	ANP	400	40.747	72.594	1.026	1	38.52
5230	C6	ANP	400	40.343	71.534	0.249	1	38.14
5231	N6	ANP	400	41.13	70.37	0.215	1	36.43
5232	N1	ANP	400	39.205	71.689	-0.435	1	34.26
5233	C2	ANP	400	38.426	72.775	-0.424	1	33.3
5234	N3	ANP	400	38.699	73.876	0.283	1	34.84
5235	C4	ANP	400	39.852	73.774	0.992	1	38.04
5236	PG	ANP	1400	4.1	35.932	42.968	1	63.65
5237	O1G	ANP	1400	2.553	36.103	43.102	1	65.57
5238	O2G	ANP	1400	4.654	37.138	42.145	1	64.12
5239	O3G	ANP	1400	4.313	34.574	42.221	1	61.2
5240	PB	ANP	1400	4.902	34.747	45.367	1	56.74
5241	O1B	ANP	1400	3.744	34.632	46.371	1	55.92
5242	O2B	ANP	1400	5.312	33.508	44.575	1	48.81
5243	N3B	ANP	1400	4.635	35.94	44.396	1	57.4
5244	PA	ANP	1400	7.146	36.343	46.365	1	46.37
5245	O1A	ANP	1400	8.575	35.772	46.69	1	41.77
5246	O2A	ANP	1400	7.182	36.981	45.004	1	44.73
5247	O3A	ANP	1400	6.043	35.092	46.457	1	48.88
5248	O5*	ANP	1400	6.76	37.46	47.388	1	45.77
5249	C5*	ANP	1400	5.479	38.164	47.395	1	40.76
5250	C4*	ANP	1400	5.665	39.356	48.337	1	40.9
5251	O4*	ANP	1400	6.474	38.947	49.45	1	41.82
5252	C3*	ANP	1400	6.555	40.431	47.668	1	41.24
5253	O3*	ANP	1400	5.736	41.351	47.02	1	46.65
5254	C2*	ANP	1400	7.326	41.125	48.784	1	40.23
5255	O2*	ANP	1400	6.547	42.006	49.545	1	40.94
5256	C1*	ANP	1400	7.516	39.913	49.694	1	40.13
5257	N9	ANP	1400	8.832	39.467	49.865	1	37.04
5258	C8	ANP	1400	9.337	38.312	49.355	1	37.62
5259	N7	ANP	1400	10.61	38.124	49.741	1	37.12
5260	C5	ANP	1400	10.899	39.2	50.517	1	37.85
5261	C6	ANP	1400	12	39.606	51.214	1	38.14
5262	N6	ANP	1400	13.153	38.775	51.202	1	37.1
5263	N1	ANP	1400	11.9	40.764	51.885	1	33.25
5264	C2	ANP	1400	10.832	41.541	51.928	1	37.47

Figure 1

Atom	Atom Type	Residue	#	X	Y	Z	OCC	B
5265	N3	ANP	1400	9.684	41.246	51.287	1	37.53
5266	C4	ANP	1400	9.738	40.091	50.598	1	38.23
5267	O	HOH	2001	10.772	33.949	38.425	1	20.93
5268	O	HOH	2002	11.149	35.798	47.426	1	53.18
5269	O	HOH	2003	4.345	32.079	15.738	1	42.11
5270	O	HOH	2004	0.607	32.578	20.617	1	57.85
5271	O	HOH	2005	8.734	39.595	29.215	1	50.93
5272	O	HOH	2006	46.414	71.498	5.513	1	42.98
5273	O	HOH	2007	30.063	54.37	17.201	1	28.45
5274	O	HOH	2008	39.779	73.86	22.407	1	30.88
5275	O	HOH	2009	10.057	27.917	37.313	1	56.75
5276	O	HOH	2010	48.313	76.556	26.783	1	56.09
5277	O	HOH	2012	12.176	33.756	46.036	1	33.09
5278	O	HOH	2013	52.858	64.574	-9.851	1	35.64
5279	O	HOH	2014	5.85	31.615	25.114	1	44.11
5280	O	HOH	2015	35.374	78.198	23.486	1	65.59
5281	O	HOH	2016	6.755	30.619	44.678	1	38.97
5282	O	HOH	2017	47.846	63.253	-11.777	1	36.83
5283	O	HOH	2018	31.706	81.437	14.674	1	48.14
5284	O	HOH	2020	51.835	72.941	13.996	1	36.01
5285	O	HOH	2021	9.15	31.445	69.292	1	39.65
5286	O	HOH	2022	47.091	66.467	-8.015	1	43.66
5287	O	HOH	2023	29.609	71.817	-0.007	1	38.11
5288	O	HOH	2024	18.734	27.61	60.73	1	44.58
5289	O	HOH	2025	6.819	36.938	69.156	1	50.09
5290	O	HOH	2026	2.441	47.624	10.242	1	57.1
5291	O	HOH	2027	3.003	42.903	46.921	1	53.16
5292	O	HOH	2028	54.131	76.111	18.046	1	47.63
5293	O	HOH	2029	23.493	21.71	48.962	1	60.57
5294	O	HOH	2030	60.032	80.82	3.634	1	84.88
5295	O	HOH	2031	27.727	81.623	12.559	1	38.04
5296	O	HOH	2032	1.909	52.215	39.067	1	44.72
5297	O	HOH	2033	-2.186	21.394	40.979	1	89.31
5298	O	HOH	2034	20.499	33.652	45.278	1	41.5
5299	O	HOH	2035	34.06	80.711	41.447	1	100
5300	O	HOH	2036	2.839	48.517	40.091	1	41.86
5301	O	HOH	2037	3.517	31.703	45.521	1	64.44
5302	O	HOH	2038	9.385	64.924	27.742	1	81.27
5303	O	HOH	2039	40.448	79.937	8.562	1	59.32
5304	O	HOH	2040	24.866	85.129	6.506	1	52.79
5305	O	HOH	2041	42.662	69.456	27.547	1	33.54
5306	O	HOH	2042	45.974	72.478	13.009	1	45.87
5307	O	HOH	2043	10.504	38.973	33.547	1	40.02
5308	O	HOH	2044	9.579	41.828	67.318	1	59.9
5309	O	HOH	2045	17.341	33.54	19.641	1	45.32
5310	O	HOH	2046	3.405	47.845	31.275	1	36.21
5311	O	HOH	2047	17.011	33.897	71.868	1	33.52
5312	O	HOH	2048	6.482	40.003	35.841	1	57.08
5313	O	HOH	2049	1.137	33.078	34.05	1	33.82
5314	O	HOH	2050	26.744	31.01	39.861	1	55.08
5315	O	HOH	2051	0.17	38.998	26.667	1	38.22
5316	O	HOH	2052	32.319	78.969	20.662	1	35.9
5317	O	HOH	2053	8.371	43.433	51.842	1	48.92
5318	O	HOH	2054	3.561	26.075	27.401	1	48.98
5319	O	HOH	2055	47.329	81.696	30.891	1	46.24
5320	O	HOH	2056	10.866	35.347	9.28	1	84.73

Figure 1

Atom	Atom Type	Residue	#	X	Y	Z	OCC	B
5321	O	HOH	2057	16.156	77.623	24.389	1	68.54
5322	O	HOH	2058	55.244	60.234	8.553	1	42.78
5323	O	HOH	2059	39.091	58.612	21.163	1	48.48
5324	O	HOH	2060	8.065	40.362	61.751	1	43.34
5325	O	HOH	2061	5.215	43.203	58.214	1	38.27
5326	O	HOH	2062	4.37	44.153	28.361	1	57.63
5327	O	HOH	2063	48.26	61.512	-6.32	1	42.92
5328	O	HOH	2064	55.392	69.84	-13.305	1	44.52
5329	O	HOH	2065	6.363	15.594	60.437	1	54.58
5330	O	HOH	2066	40.18	75.691	-10.457	1	41.92
5331	O	HOH	2067	39.635	79.313	26.163	1	34.64
5332	O	HOH	2068	21.112	51.594	19.282	1	54.97
5333	O	HOH	2069	2.935	39.989	25.661	1	47.84
5334	O	HOH	2070	-0.739	41.793	34.308	1	51.1
5335	O	HOH	2071	-1.97	28.873	17.982	1	76.51
5336	O	HOH	2072	37.519	83.18	17.527	1	66.32
5337	O	HOH	2073	22.213	35.923	45.566	1	43.82
5338	O	HOH	2074	54.866	66.859	-13.461	1	36.44
5339	O	HOH	2075	18.985	68.519	7.218	1	53.24
5340	O	HOH	2076	33	49.476	38.019	1	66.05
5341	O	HOH	2077	1.385	19.187	61.122	1	40.14
5342	O	HOH	2078	28.317	49.852	34.842	1	61.51
5343	O	HOH	2079	58.966	69.737	-6.012	1	48
5344	O	HOH	2080	20.219	33.371	71.707	1	62.38
5345	O	HOH	2081	54.919	74.501	-19.389	1	57.57
5346	O	HOH	2082	6.715	29.888	73.444	1	46.38
5347	O	HOH	2083	34.395	81.934	13.78	1	52.33
5348	O	HOH	2084	4.674	31.598	71.807	1	58.4
5349	O	HOH	2085	53.164	70.664	-14.524	1	63.38
5350	O	HOH	2086	45.625	80.173	17.79	1	55.61
5351	O	HOH	2087	12.941	37.096	23.879	1	63.59
5352	O	HOH	2088	38.14	82.799	2.37	1	48.54
5353	O	HOH	2089	48.766	66.048	26.928	1	52.02
5354	O	HOH	2090	52.39	79.487	6.131	1	76.26
5355	O	HOH	2091	0.174	21.376	54.024	1	60.77
5356	O	HOH	2092	50.341	82.455	0.703	1	74.32
5357	O	HOH	2093	64.689	80.903	3.248	1	53.52
5358	O	HOH	2094	-1.36	44.694	7.571	1	71.2
5359	O	HOH	2095	23.367	50.964	52.62	1	67.99
5360	O	HOH	2096	-6.492	34.887	17.192	1	56.94
5361	O	HOH	2097	3.543	36.942	38.901	1	63.66
5362	O	HOH	2098	-6.969	32.565	62.065	1	84.57
5363	O	HOH	2099	27.25	53.447	25.318	1	41.81
5364	O	HOH	2100	8.338	49.512	14.509	1	38.78
5365	O	HOH	2101	26.169	41.831	37.281	1	46.37
5366	O	HOH	2102	12.608	35.089	21.09	1	42.82
5367	O	HOH	2103	13.632	23.185	63.6	1	42.07
5368	O	HOH	2104	54.824	68.31	25.143	1	74.51
5369	O	HOH	2105	19.642	22.43	33.592	1	54.13
5370	O	HOH	2106	45.757	62.224	5.571	1	50.62
5371	O	HOH	2107	19.587	35.893	72.506	1	46.36
5372	O	HOH	2108	3.087	45.759	45.5	1	60.82
5373	O	HOH	2109	15.907	57.243	21.733	1	54.68
5374	O	HOH	2110	48.651	56.028	10.536	1	95.92
5375	O	HOH	2111	44.053	79.03	12.315	1	58.92
5376	O	HOH	2112	29.827	77.335	39.215	1	63.64

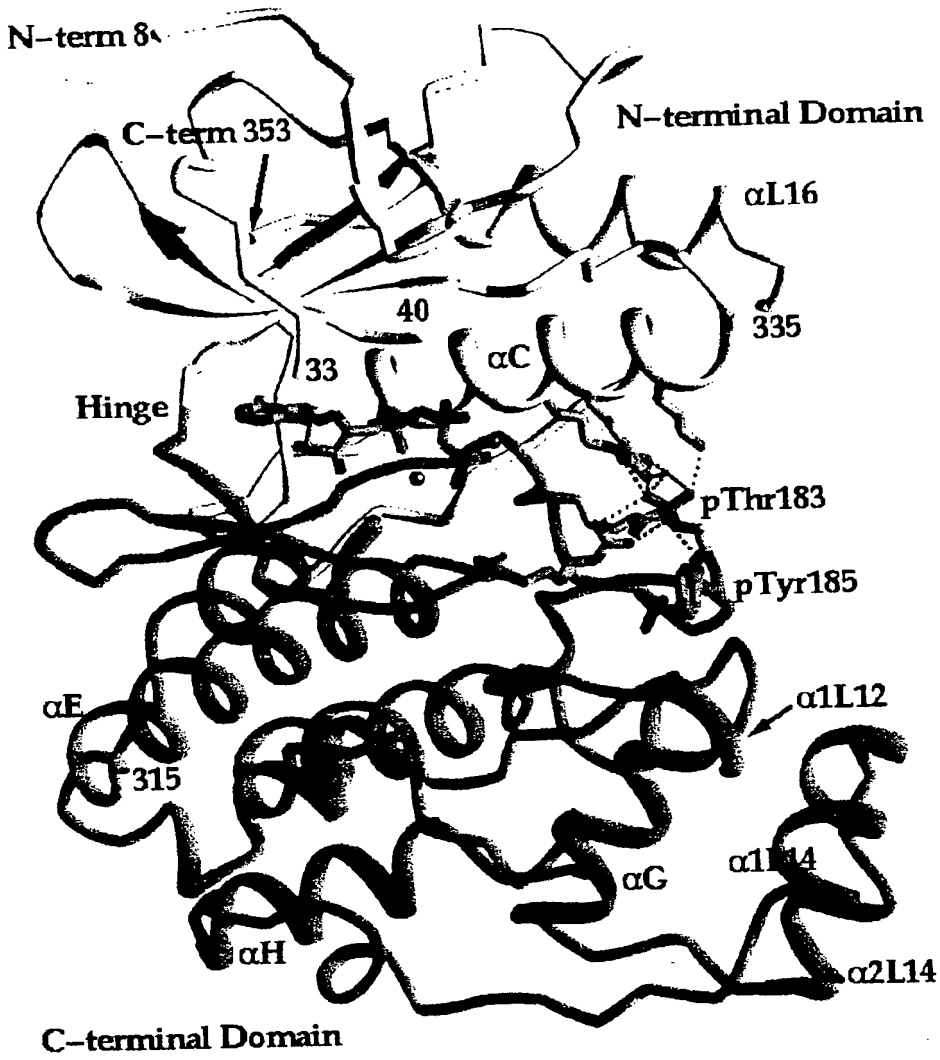
Figure 1

Atom	Atom Type	Residue	#	X	Y	Z	OCC	B
5377	O	HOH	2113	15.946	37.221	20.809	1	89.1
5378	O	HOH	2114	10.008	22.941	31.02	1	48.95
5379	O	HOH	2115	24.846	86.734	4.358	1	51.7
5380	O	HOH	2116	4.595	49.482	33.513	1	67.71
5381	O	HOH	2117	0.793	45.008	38.422	1	50.43
5382	O	HOH	2118	6.692	33.791	39.701	1	50.68
5383	O	HOH	2119	9.649	48.935	19.05	1	68.49
5384	O	HOH	2120	40.249	75.205	51.582	1	51.92
5385	O	HOH	2121	51.66	60.888	21.709	1	53.75
5386	O	HOH	2122	39.346	57.224	24.107	1	46.15
5387	O	HOH	2123	31.728	42.838	36.454	1	44.17
5388	O	HOH	2124	40.051	76.285	16.447	1	79.22
5389	O	HOH	2125	31.248	77.875	18.437	1	66.18
5390	O	HOH	2126	13.547	60.547	17.434	1	57.4
5391	O	HOH	2127	11.489	54.75	50.23	1	76.19
5392	O	HOH	2128	20.054	55.492	50.224	1	37.59
5393	O	HOH	2129	17.42	30.752	70.714	1	40.8
5394	O	HOH	2130	18.168	33.914	60.155	1	34.83
5395	O	HOH	2131	18.744	75.66	19.427	1	46.31
5396	O	HOH	2132	20.991	40.391	29.318	1	59.96
5397	O	HOH	2133	40.93	81.758	25.48	1	48.17
5398	O	HOH	2134	29.094	49.017	42.215	1	43.78
5399	O	HOH	2135	16.41	23.271	37.302	1	64.3
5400	O	HOH	2136	40.832	72.121	18.068	1	62.51
5401	O	HOH	2137	3.713	54.002	31.916	1	51.43
5402	O	HOH	2138	6.52	25.87	33.79	1	74.01
5403	O	HOH	2139	0.338	30.422	52.543	1	60.63
5404	O	HOH	2140	0.144	40.98	46.433	1	55.17
5405	O	HOH	2141	19.662	78.537	20.473	1	53
5406	O	HOH	2142	45.784	57.815	-8.304	1	59.05
5407	O	HOH	2143	27.448	43.857	38.986	1	80.17
5408	O	HOH	2144	24.726	83.636	2.342	1	49.9
5409	O	HOH	2145	11.951	55.373	53.119	1	48.01
5410	O	HOH	2146	14.632	47.119	60.154	1	59.79
5411	O	HOH	2147	-1.117	38.112	34.017	1	36.44
5412	O	HOH	2148	24.72	59.34	35.09	1	62.65
5413	O	HOH	2149	7.817	29.839	18.139	1	52.06
5414	O	HOH	2150	13.577	26.758	66.33	1	55.54
5415	O	HOH	2151	-4.626	35.494	34.477	1	54.33
5416	O	HOH	2152	48.764	76.038	7.667	1	45.14
5417	O	HOH	2153	45.78	76.292	11.913	1	48.89
5418	O	HOH	2154	65.621	78.088	14.103	1	87.09
5419	O	HOH	2155	14.776	33.227	20.254	1	53.71
5420	O	HOH	2156	-6.492	47.579	23.192	1	71.61
5421	O	HOH	2157	10.912	36.446	19.347	1	71.91
5422	O	HOH	2158	-0.483	27.212	15.775	1	52.36
5423	O	HOH	2159	57.616	59.487	20.576	1	52.03
5424	O	HOH	2160	11.348	23.02	17.901	1	58.83
5425	O	HOH	2161	6.859	33.83	69.706	1	49.25
5426	O	HOH	2162	21.464	66.188	29.151	1	40.81
5427	O	HOH	2163	12.695	66.769	14.259	1	60.77
5428	O	HOH	2164	1.375	47.587	37.345	1	71.1
5429	O	HOH	2165	28.494	41.431	39.072	1	56.88
5430	O	HOH	2166	38.323	73.53	35.555	1	58.84
5431	O	HOH	2167	22.536	44.887	51.419	1	70.03
5432	O	HOH	2168	28.691	82.952	26.989	1	43.85

Figure 1

Atom	Atom Type	Residue	#	X	Y	Z	OCC	B
5433	O	HOH	2169	44.743	80.266	-14.044	1	78.59
5434	O	HOH	2170	3.922	45.869	19.001	1	96.76
5435	O	HOH	2171	57.137	69.168	23.44	1	61.66
5436	O	HOH	2172	28.574	78.161	18.537	1	100
5437	O	HOH	2173	55.573	65.877	-11.131	1	58.89
5438	O	HOH	2174	7	18.47	63.559	1	52.76
5439	O	HOH	2175	-0.497	29.47	10.663	1	65.7
5440	O	HOH	2176	39.55	62.054	21.834	1	69.36
5441	O	HOH	2177	48.756	83.508	29.35	1	62.82
5442	O	HOH	2178	7.812	62.749	20.621	1	67.61
5443	O	HOH	2179	9.736	47.516	63.408	1	46.59
5444	O	HOH	2180	36.458	90.23	30.756	1	75.67
5445	O	HOH	2181	32.054	74.879	38.041	1	49.33
5446	O	HOH	2182	25.001	46.519	52.531	1	64.94
5447	O	HOH	2183	32.47	79.959	12.122	1	56.23
5448	O	HOH	2184	-7.077	43.484	33.181	1	56.09
5449	O	HOH	2185	2.143	38.605	42.272	1	53.31
5450	O	HOH	2186	6.04	44.393	50.82	1	92.01
5451	O	HOH	2187	20.678	35.691	62.368	1	55.76
5452	O	HOH	2188	6.896	24.913	15.884	1	61.33

Figure 1a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C-terminal Domain

Figure 2

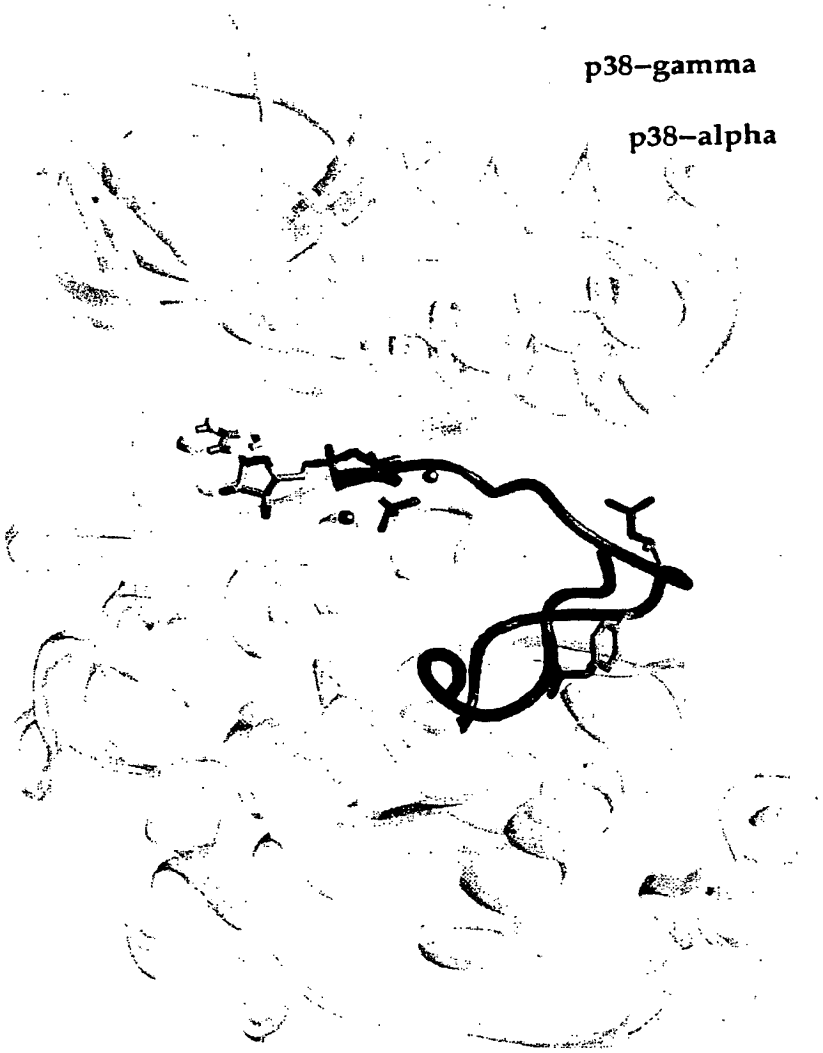
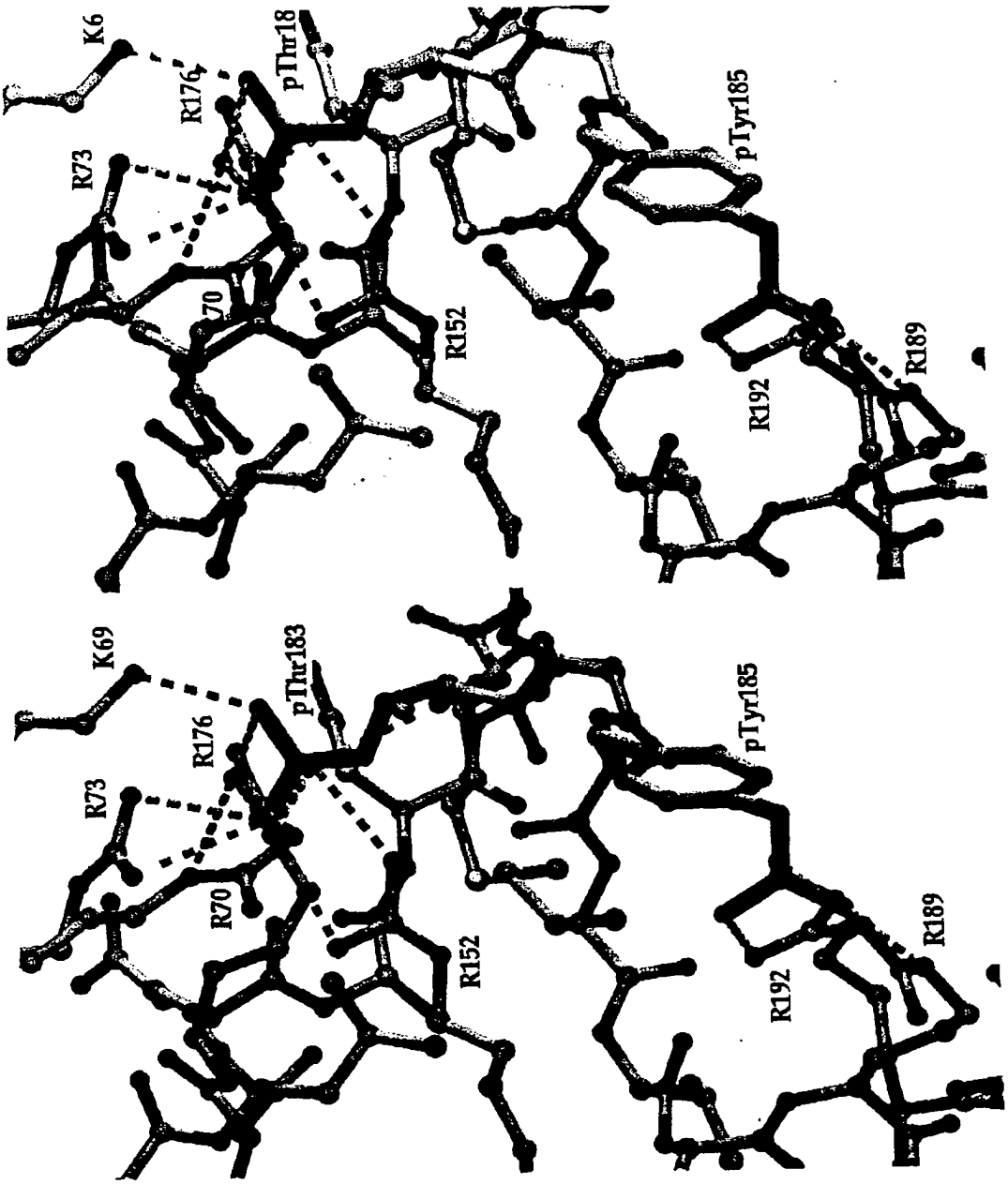


Figure 3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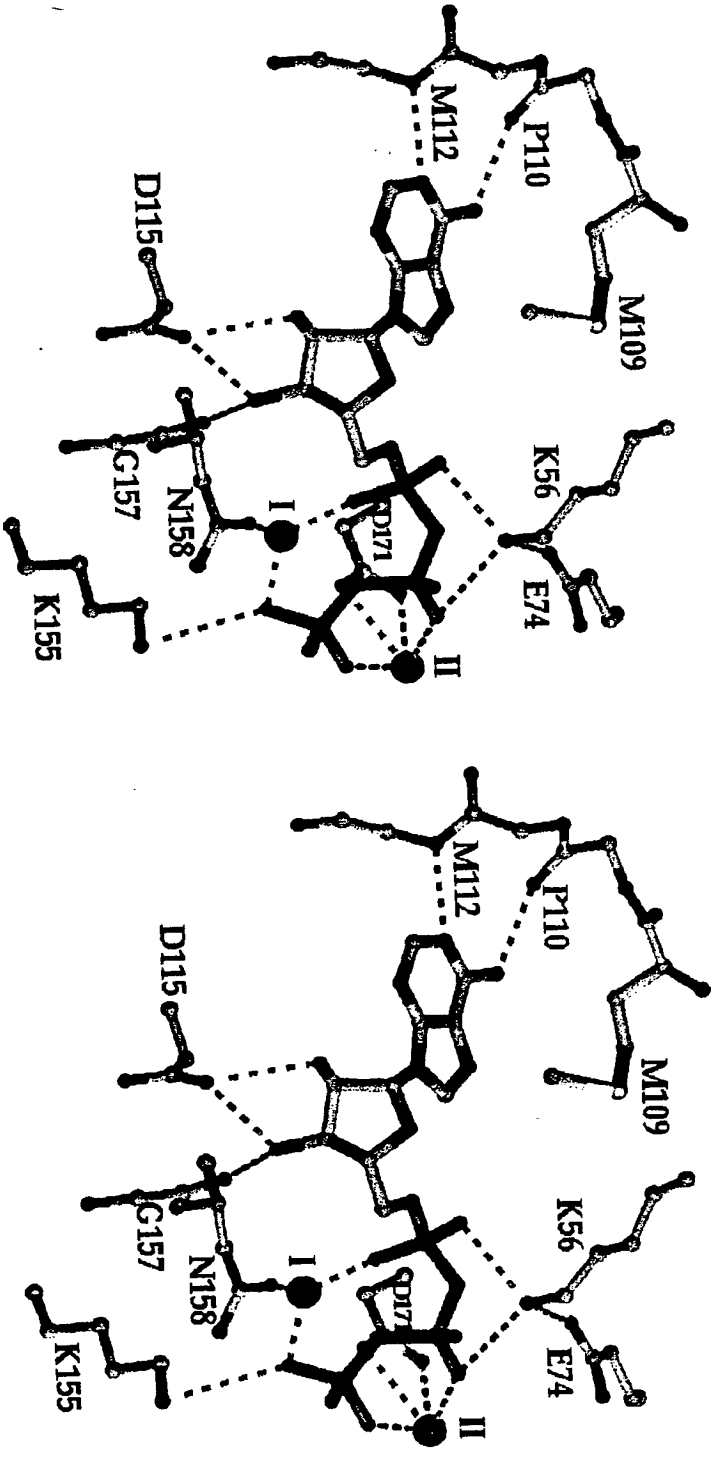
R152
pTyr185
R192
R189

3.

Figure 4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P110
D115
M109
G157
N158
I
D171
K56
K155
E74
II
M112
P110
D115
M109
G157
N158
I
D171
K56
K155
E74
II

Figure 5A

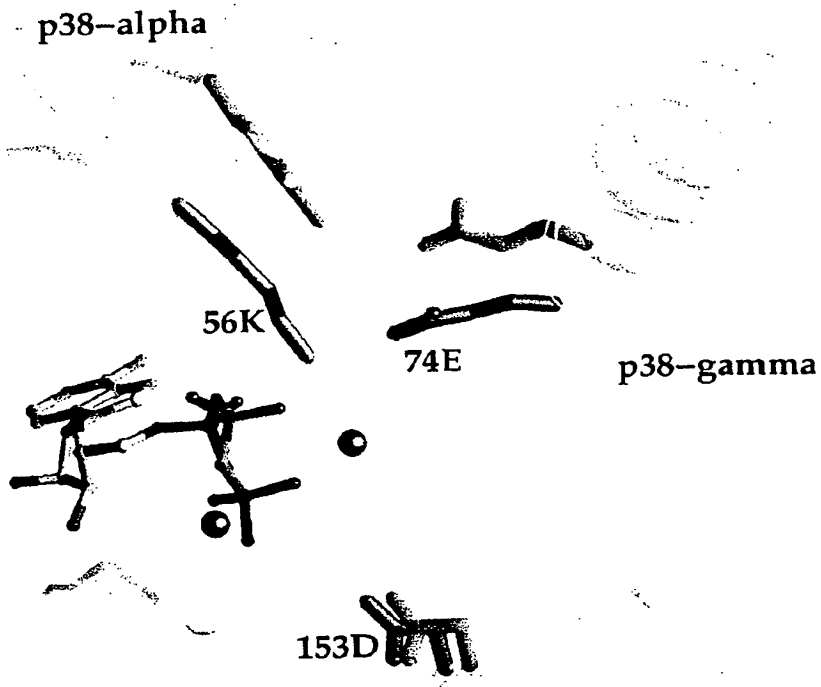


Figure 5B

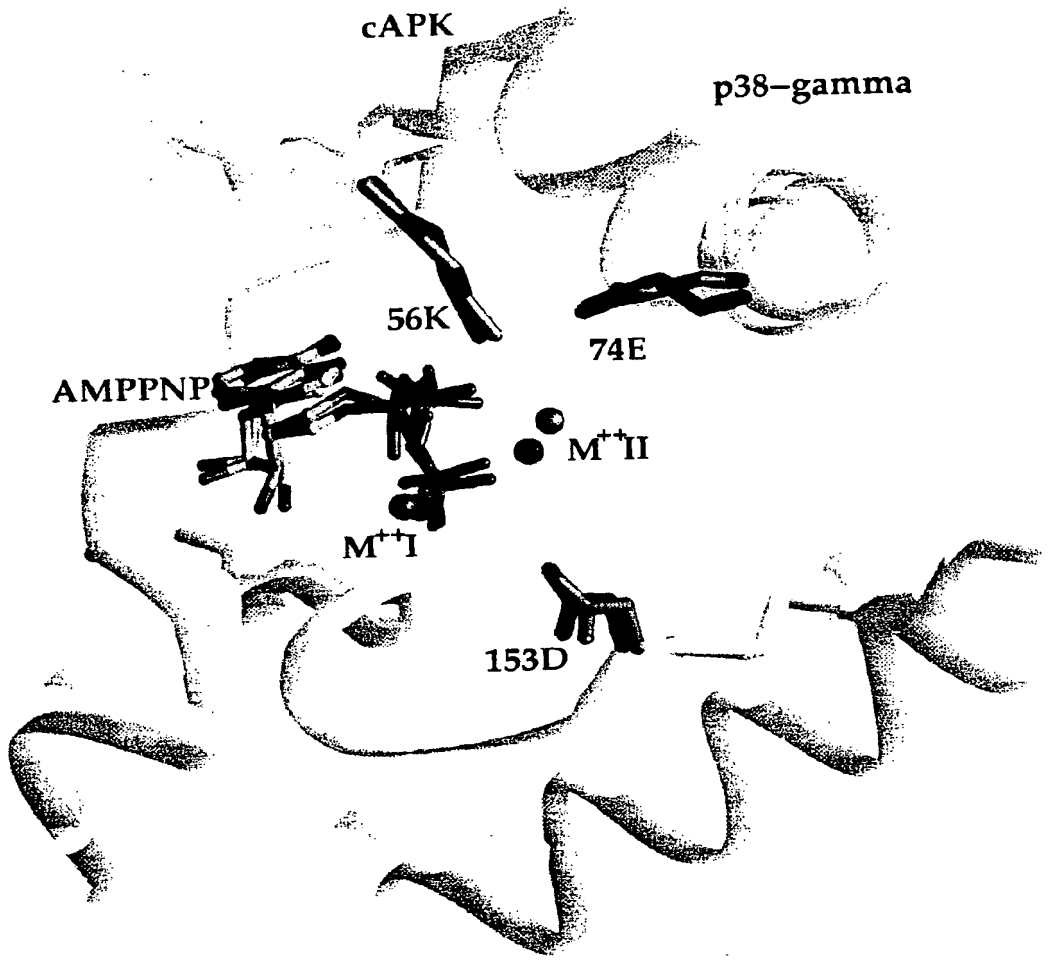


FIGURE 6

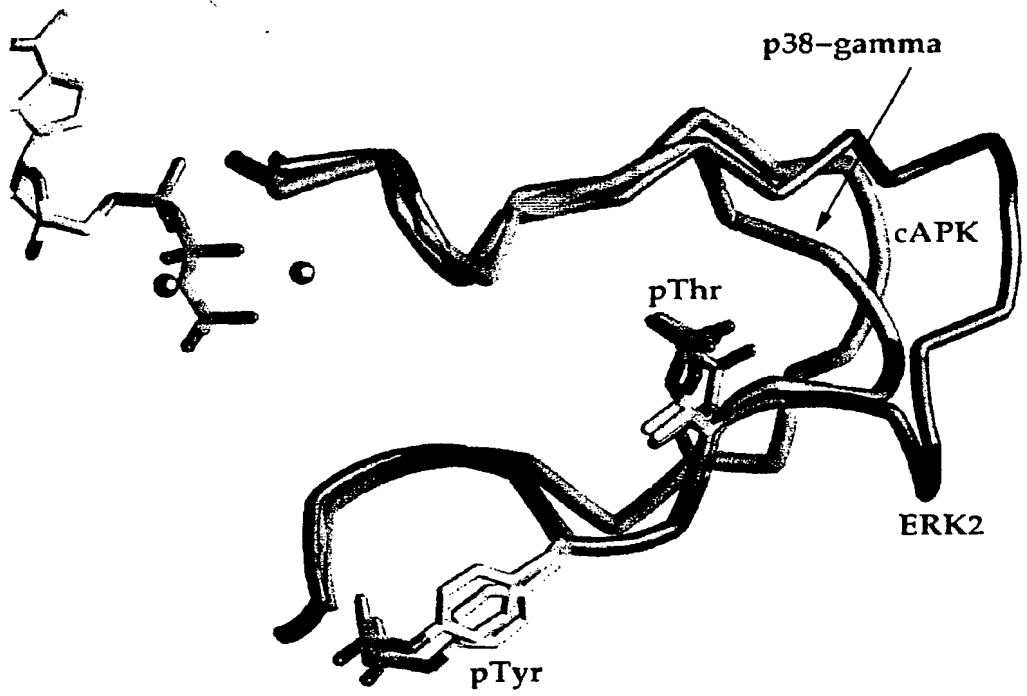
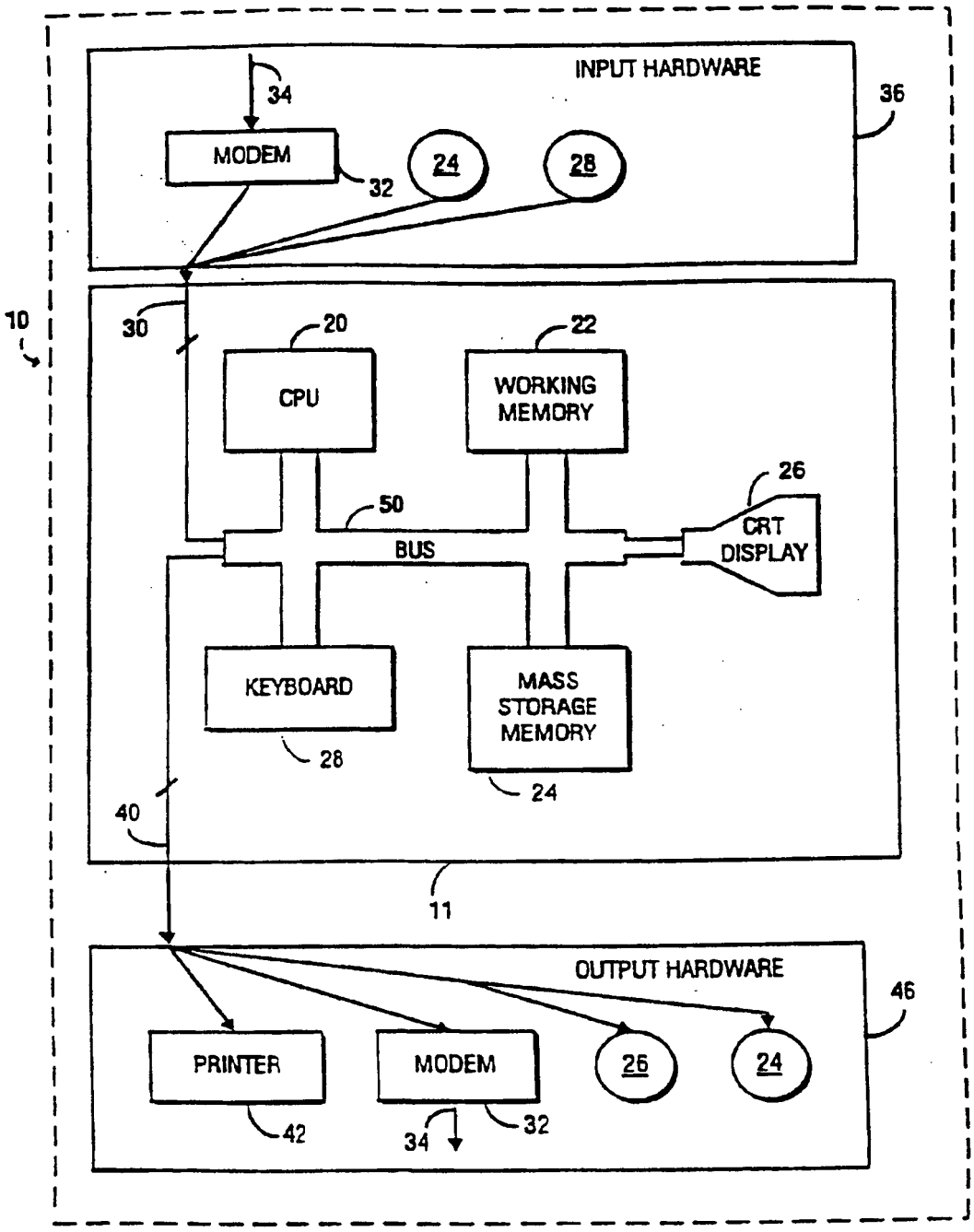


FIGURE 7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36
MODEM
32
24
28
10
30
20
22
CPU
WORKING MEMORY
26
50
CRT DISPLAY
BUS
KEYBOARD
MASS STORAGE MEMORY
28
24
40
11
OUTPUT HARDWARE
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PRINTER
MODEM
26
24
42
34
32

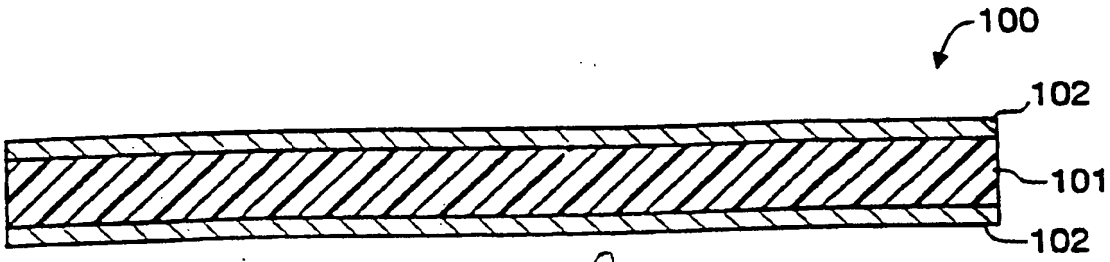

FIGURE 8

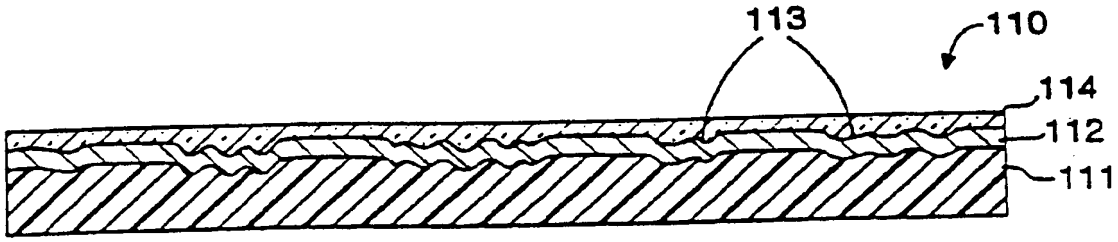

FIGURE 9

INTERNATIONAL SEARCH REPORT

Inter nal Application No
PCT/US 99/29096

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C12N9/12 G01N23/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C12N G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	MERTENS S ET AL: "SAP KINASE-3, A NEW MEMBER OF THE FAMILY OF MAMMALIAN STRESS-ACTIVATED PROTEIN KINASES" FEBS LETTERS,NL,ELSEVIER SCIENCE PUBLISHERS, AMSTERDAM, vol. 383, 1 January 1996 (1996-01-01), pages 273-276, XP002053847 ISSN: 0014-5793 the whole document	1-6
X	LI Z. ET AL.: "The primary structure of p38-gamma: a new member of 38 group of MAP kinases" BIOCHEM. BIOPHYS. RES. COM., vol. 228, 1996, pages 334-340, XP002041225	1-6
Y	the whole document	7-17
	-/--	

[X] Further documents are listed in the continuation of box C.

[ ] Patent family members are listed in annex.

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"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
15 May 2000	25/05/2000

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Panzica, G

2

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
Y	BÖHM H -J: "THE COMPUTER PROGRAM LUDI: A NEW METHOD FOR THE DE NOVO DESIGN OF ENZYME INHIBITORS" JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN,XX,ESCOM SCIENCE PUBLISHERS BV, vol. 11, no. 2, August 1991 (1991-08), pages 61-78, XP002914895 ISSN: 0920-654X cited in the application the whole document	7-17
A	GHOSE A K ET AL: "DETERMINATION OF PHARMACOPHORIC GEOMETRY FOR COLLAGENASE INHIBITORSDETERMINATION OF PHARMACOPHORIC GEOMETRY FOR COLLAGENASE INHIBITORSUSING A NOVEL COMPUTATIONAL METHOD AND ITS VERIFICATION USING USING A NOVEL COMPUTATIONAL METHOD AND ITS VERIFICATION USING MOLECULAR DYNAMICS, NMR, AND X-RAY CRYSTAL" JOURNAL OF THE AMERICAN CHEMICAL SOCIETY,US,AMERICAN CHEMICAL SOCIETY, WASHINGTON, DC, vol. 117, no. 16, 1 January 1995 (1995-01-01), pages 4671-4682-467, XP002051616 ISSN: 0002-7863 the whole document	7-17
X	GOEDERT M ET AL.: "Phosphorylation of microtubule-associated protein tau by stress-activated protein kinases" FEBS LETTERS, vol. 409, 1997, pages 57-62, XP000906954 AMSTERDAM NL the whole document	1-6
X	KUMAR S. ET AL.: "Novel homologous of CSBP/p38 MAP kinase: activation, substrate specificity adn sensitivity to inhibition by pyrydinyl imidazoles" BIOCHEM. BIOPHYS. RES. COM., vol. 235, 1997, pages 533-538, XP002041227 the whole document	1-6
X	KEESLER G. ET AL.: "Purification and activation of recombinant p38 isoforms alpha, beta, gamma and delta" PROTEIN EXPRESSION AND PURIFICATION, vol. 14, November 1998 (1998-11), pages 221-228, XP000909191 the whole document	1-6

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2

INTERNATIONAL SEARCH REPORT

Intern .nal Application No
PCT/US 99/29096

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
X,P	BELLON S. ET AL.: "The structure of phosphorylated P38gamma is monomeric and reveals a conserved activation-loop conformation" STRUCTURE, vol. 7, 15 September 1999 (1999-09-15), pages 1057-1065, XP000909285 the whole document	1-17

2

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